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User's Manual for OZIPM-2
Ozone Isopleth Plotting with Optional Mechanisms/Version 2

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User's Manual For OZIPM-2: Ozone Isopleth Plotting With Optional Mechanisms/ Version 2

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16. ABSTRACT

Ozone Isopleth Plotting with Optional Mechanisms/Version 2 (OZIPM-2) is a computerized model that simulates ozone formation in urban atmospheres. OZIPM-2 calculates maximum one-hour average ozone concentrations given a set of input assumptions about initial precursor concentrations, light intensity, dilution, diurnal and spatial emission patterns, transported pollutant concentrations, and reactivity of the precursor mix. OZIPM-2 also accepts as input any user supplied chemical mechanism. The results of multiple simulations are used to produce an ozone isopleth diagram tailored to particular cities. Such a diagram relates maximum ozone concentrations to concentrations of non-methane organic compounds and oxides of nitrogen, and can be used in the Empirical Kinetic Modeling Approach (EKMA) to calculate the emission reductions necessary to achieve air quality standards for photochemical oxidants. This user's manual describes the technical basis, necessary and optional input data, computer code and the use of OZIPM-2.

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User's Manual For OZIPM-2: Ozone Isopleth Plotting With Optional Mechanisms/Version 2

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August 1984

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PREFACE

This publication contains information on the OZIPM-2 computer program. Although the program has been checked throughly on a UNIVAC computing system, incompatibilities on other systems may be found. In case there is a need to update this program, revisions will be distributed in the same manner as this report. Revisions may also be obtained as they are issued by completing and mailing the form at the front of the manual.

The computer program described in this manual is available from the U. S. Environmental Protection Agency, and can be acquired by sending a magnetic tape along with a written request to:

OZIPM-2 Program
Air Management Technology Branch (MD-14)
Monitoring and Data Analysis Division
U. S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

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1.0 INTRODUCTION

The Empirical Kinetics Modeling Approach (EKMA) is a procedure for evaluating what effect changes in emissions of Volatile Organic Compounds (VOC) and oxides of nitrogen (NO_x) will have on ambient concentrations of ozone.[1,2,3,4] The evaluations are carried out by using ozone isopleth diagrams that graphically depict peak, one-hour average concentrations of ozone as a function of early-morning concentrations of nonmethane organic compounds (NMOC) and NO_x. The isopleth diagrams can be generated by a computer program known as the Kinetics Model and Ozone Isopleth Plotting Package, or OZIPP.[5,6] In constructing these diagrams, OZIPP makes use of a simplified trajectory model and a chemical kinetic mechanism developed by Dodge that mathematically simulate the atmospheric processes leading to the formation of ozone and other by-products.[2] With the advent of newer chemical mechanisms, the need has arisen for a more general program that allows the use of alternate mechanisms. One such program, Ozone Isopleth Plotting with Optional Mechanisms (OZIPM), has been available for some time.[7] Since its development, a number of revisions have been made to the computer code in an effort to improve its flexibility and to enhance its compatability among various computer systems. The purpose of this manual is to describe the revised computer program, its associated input requirements, output generated by the program and some computer considerations that should be taken into account when executing the program. To avoid confusion with the previous version of OZIPM, the new program will be referred to as OZIPM/Version 2, or OZIPM-2.

Those familiar with the original OZIPM program know that it is operationally similar to OZIPP, the program designed to be used exclusively with the DODGE mechanism. This same operational structure has been retained in OZIPM-2. Because the theoretical basis for OZIPM-2 and OZIPP is the same, and because both models operate in a similar manner, the descriptions of each overlap considerably. As a consequence, most emphasis in this document will be placed on describing the new options that have been incorporated in OZIPM-2. For those unfamiliar with either OZIPP or OZIPM, the use of Reference 6, User's Manual For Kinetics Model and Ozone Isopleth Plotting Package, as a companion document to this manual is recommended. Finally, it should be emphasized that this document is directed primarily towards those who are involved in coding input data and setting up the computer runs. For information on how the model inputs are formulated and how the model results can be used in typical regulatory applications, the reader is referred to documents such as References 8 and 9.

The remaining portions of this chapter are divided into three sections. The first provides a general overview of the OZIPM-2 model, with particular emphasis placed on summarizing differences between OZIPM-2 and OZIPP. This section is followed by brief discussions of OZIPM-2 structure, required input data, and the output produced by the program. The remaining chapters discuss the technical basis for the model, the program options, and the procedures for formatting input data and running the model. The final chapter includes example model runs illustrating the concepts discussed in the previous chapters.

1.1 MODEL OVERVIEW

As noted previously, the EKMA technique makes use of ozone isopleth diagrams to relate changes in peak ozone concentration to changes in VOC and/or NO_x emissions. As such, it is primarily intended for estimating emission controls that are needed within an urban area as part of the State Implementation Plans (SIPs) to achieve the National Ambient Air Quality Standard (NAAQS) for ozone. EKMA is therefore most appropriately used to address the following two types of questions:

° What percentage reduction in VOC emissions will be needed to attain the NAAQS for ozone?

° What change in ozone is likely to accompany a given change in VOC emissions?

The isopleth diagrams that are generated by either OZIPP or OZIPM-2 can be made to reflect conditions that are specific to any particular urban area. Generation of these city-specific diagrams requires the use of city-specific information on the location and time of year (determining sunlight intensity), local atmospheric dilution rates, diurnal patterns of VOC and NO_x emissions, and information on pollutants transported into the city from upwind areas. The two programs can also be used to simulate the formation of a single ozone peak for a specified set of city-specific assumptions and initial concentrations of NMOC and NO_x. In this mode, the program can display the time rate of change in pollutant concentrations, as well as rates of individual chemical reactions. In either the isopleth or single simulation mode, the models are generally limited in applicability to ozone problems within or immediately downwind of urban areas, and thus, not applicable to the following types of situations:

° rural ozone problems

° cases in which peak ozone occurs very early in the morning or at night

° development of control strategies for single sources or small groups of sources.

The theoretical model underlying both OZIPP and OZIPM-2 is conceptually similar to a trajectory-type photochemical simulation model. A column of air contains initial concentrations of ozone and its precursors. The height of the column extends from the earth's surface to the top of the surface-based mixed layer, and the diameter of the column is chosen such that (1) pollutant concentrations inside and just outside the column are similar so that the horizontal exchange of the air at the perimeter of the column can be ignored, and (2) the horizontal exchange at the column's boundaries is small compared to the volume of air within the column. The column moves along a user-defined trajectory, picking up fresh emissions which are dispersed uniformly and instantaneously throughout the column. Also as the column moves, the mixed layer (i.e., the column height) increases, resulting in the dilution of pollutant concentrations within the column and the entrainment of pollutants from aloft into the column. As all of these physical processes are occuring, the chemical kinetics mechanism is used to simulate the chemical reactions taking place within the column.

As noted earlier, the chemical reactions are simulated in OZIPP by means of the DODGE chemical mechanism shown in Appendix A. While OZIPM-2 also contains this mechanism as a default, a major feature of this program is that it allows the use of an alternative mechanism, and a substantial portion of this document will be directed towards describing this option.

Another new feature of OZIPM-2 is the inclusion of a routine that uses the EKMA technique to calculate directly VOC emission reductions needed to lower peak ozone to the level of the ozone NAAQS (currently, 0.12 ppm). This new option bypasses the need to generate ozone isopleth diagrams and then manually compute control estimates. Although this option does not provide as much information as the isopleth diagram, it is typically more efficient in terms of computer time. Other features of OZIPM-2 that enhance its flexibility and facilitate its routine application include the following:

° an option that allows the user to specify the diurnal growth pattern in the mixed layer;

° an option that permits the user to supply the program with information needed to compute hourly emission fractions directly rather than computing them manually; and

° options that permit specifying the composition of pollutants transported into an urban area.

1.2 SYSTEM DESCRIPTION

The system structure of OZIPM-2 is almost identical to that of OZIPP (see Figure 1-1). The program receives card-image input, and produces line printer output. Two optional output files may also be generated by the user. The first is an output file that contains the data needed to produce an isopleth diagram on an off-line plotter such as CALCOMP or VERSATEC. The second file contains information on the change in ozone as a function of VOC emission reduction that is produced by the new EKMA routine.

Internally, the structures of OZIPM-2 and OZIPP are also similar. A simulation section controls the individual model simulations, and an interpolation and plotting section controls the generation of isopleth diagrams. In addition to these two sections, OZIPM-2 also contains a new section to direct the VOC control calculations performed with the EKMA routine. The EKMA routine is described in Chapter 2, but users desiring more information on the simulation section and the interpolation and plotting section are referred to Reference 6, the OZIPP User's Manual.

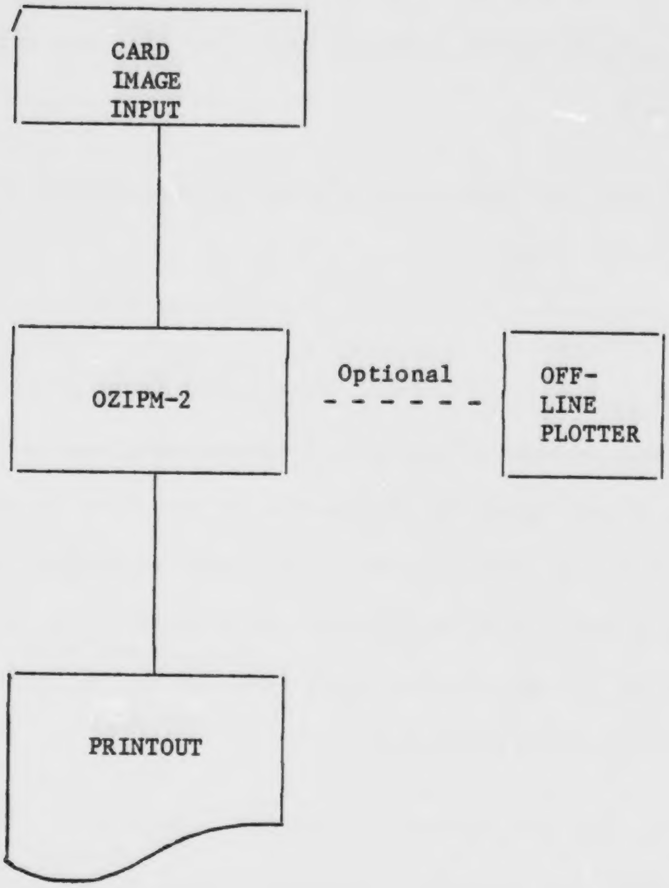

Figure 1-1. Schematic of OZIPM-2 System

1.3 INPUT/OUTPUT DATA

The OZIPM-2 program contains preset data that must generally be overridden when a city-specific diagram, EKMA calculation or single simulation is performed. Typically, these values will include:

- city latitude
- city longitude
- time zone
- date
- morning and afternoon mixing heights
- concentrations of ozone, NMOC and/or NO_x in the air above the early morning mixing height
- concentrations of ozone, NMOC and/or NO_x within the early morning mixed layer that are transported from upwind of the city
- emissions of VOC and/or NO_x after 0800 LDT
- organic reactivity
- initial fraction of NO_x that is NO_2

If a chemical mechanism other than the default is used, then additional input variables are required. Examples include identification of the organic components, proper specification of the photolytic reaction rates, and specification of the individual mechanism reactions and their corresponding rates of reaction. Additional input information is also required for the EKMA routine, including the NMOC/NO_x ratio, the observed peak ozone concentration, and the manner in which transported pollutants are assumed to change in the future. The use of some of OZIPM-2's other new options may also require additional information. For example, if the user wishes to define the diurnal mixing height profile rather than use the default pattern, then hourly mixing heights must be input.

As with OZIPP, OZIPM-2 also allows the user to control various parameters that govern program operation (e.g., error tolerances, number of simulations performed in generating an ozone isopelth diagram, etc.).

The output of OZIPM-2 is controlled by the operational mode selected by the user. In the isopleth diagram mode, tables summarizing simulation results are produced as well as a line-printer isopleth plot. The user also has the option of generating a diagram *via* an off-line plotter such as CALCOMP. Under the single simulation mode, summary tables are routinely produced, but the user has the option of obtaining detailed information for any particular simulation (e.g., concentrations of all species, rates of individual reactions, etc.). Selection of the EKMA mode causes the generation of tabular reports summarizing the simulations performed and the information used in the control calculations. Regardless of the mode that is selected, the input information supplied by the user is displayed before the generation of other outputs.

2.0 TECHNICAL DISCUSSION

The OZIPM-2 program mathematically simulates the chemical and physical processes leading to the formation of ozone in the atmosphere. The OZIPM-2 user controls these simulations by selecting one of three major options. The first option directs the model to perform a single simulation. It might be invoked, for example, to test the model's predictive capabilities. A second option available to the user causes the generation of an isopleth diagram. An ozone isopleth diagram could, for example, be used to estimate the VOC emission reduction needed to achieve the ozone NAAQS. The third major option directs OZIPM-2 to compute a VOC emission reduction estimate directly, thereby circumventing the need to generate an ozone isopleth diagram.

Of the three options discussed above, the final two (i.e., isopleth diagram generation and direct calculation of a VOC control estimate) are essentially repeated applications of the first option (i.e., the single simulation). The basis for the single simulation is a simplified kinetics/trajectory model. The purposes of this chapter are to document the mathematical formulation of that model, and to document the other, principal computational procedures associated with each of the three major options discussed above. The discussions that follow are quite detailed, and not essential to successful formulation of model inputs and subsequent model execution. Thus, potential OZIPM-2 users may wish to read the remaining chapters before this one.

2.1 MATHEMATICAL FORMULATION OF THE OZIPM-2 KINETICS MODEL

A brief narrative description of the kinetics/trajectory model underlying OZIPM-2 was presented in Chapter 1. More extensive descriptions are contained in References 3, 6, 8, and 9. Conceptually, the model is virtually identical to the one incorporated in OZIPP, although some modifications have been made to allow the use of chemical mechanisms other than the default DODGE mechanism. Since the theoretical basis for the model is independent of the mechanism selected, the discussions that follow are structured accordingly. The procedures for implementing and using an alternative mechanism will be discussed in subsequent chapters.

The mathematical formulation of the trajectory model underlying OZIPM-2 can be summarized by the set of ordinary differential equations derived from the definitions shown in Table 2-1. Several of the terms in these equations correspond to physical processes such as dilution, entrainment of pollutants from aloft, and precursor emissions. Additional terms are required to account for increases or decreases in pollutant concentrations resulting from chemical reaction. Also, solving the set of differential equations requires that the species concentrations at the beginning of the simulation (i.e., initial concentrations) be specified. The equations in Table 2-1 are solved numerically to produce instantaneous concentrations of individual species as a function of time. OZIPM-2 also computes the maximum one-hour concentration of ozone (or any other specified pollutant) that occurs within the simulation period (normally 0800 LDT to 1800 LDT). The discussions below begin with definitions of the individual terms in the set of equations shown in Table 2-1, and conclude with descriptions of the procedures used to perform a single simulation, generate an isopleth diagram, or compute a VOC control estimate directly.

2.1.1 Initial Conditions

In any trajectory model application, concentrations of all species within the theoretical column of air must be specified for the time at which the simulation starts. Whenever a single simulation is performed with OZIPM-2, the initial concentrations of organics and NO_x must be specified by the user.

TABLE 2-1. MATHEMATICAL REPRESENTATION OF THE OZIPM-2 KINETICS/TRAJECTORY MODEL[a]

C_i = the concentrations of the ith chemical species in the mixed volume at time = t

$C_i(@0)$ = the initial concentration of the ith species in the mixed volume at time = 0

C_i^{aloft} = the concentration of the ith species above the mixed layer

$H = f(t)$	mixing height at time = t
$\frac{dH}{dt} = f'(t)$	rate of rise at time = t
$K_D = (\frac{1}{H})\frac{dH}{dt}$	dilution rate at time = t
$\left.\frac{dC_i}{dt}\right\|_{dil} = -K_D C_i$	decrease in species i caused by mixing height rise
$\left.\frac{dC_i}{dt}\right\|_{ent} = K_D C_i^{aloft}$	increase in species i caused by entrainment due to mixing height rise
$E_i = f(t)$	mass of species C_i emitted per unit time at time = t (concentration - height units)
$\left.\frac{dC_i}{dt}\right\|_{emis} = E_i/H$	increase in species C_i caused by emissions into a mixing volume with unit area and height, MH, at time t
$P_i = \text{func}(C_j, j=1,n)$	production of species C_i due to chemical formation at time t
$L_i = \text{func}(C_j, j=1,n)$	loss of species C_i due to chemical reaction at time t
$\left.\frac{dC_i}{dt}\right\|_{chem} = P_i - L_i$	increase or decrease in species C_i caused by chemical reactions of all species at time t

$$\left.\frac{dC_i}{dt}\right|_{TOTAL} = \left.\frac{dC_i}{dt}\right|_{dil} + \left.\frac{dC_i}{dt}\right|_{ent} + \left.\frac{dC_i}{dt}\right|_{emis} + \left.\frac{dC_i}{dt}\right|_{chem}$$

SOLUTION:

$$C_i = C_i(@0) + \int_0^t \left.\frac{dC_i}{dt}\right|_{TOTAL}$$

numerical integration used to solve initial value, differential equation problem

---

[a] Adopted from Reference 10.

(When utilizing the isopleth or EKMA options, however, these concentrations are generated internally by the program.) For all other species in the mechanism, default concentrations are zero, although the user has the option to override these by specifying the concentration of any individual species. In addition to the initial concentrations, the user has the option of specifying ozone, NO_x, and/or NMOC levels that are transported into the city within the surface layer. The transport levels are added to the initial concentrations to determine the overall initial concentrations used in the model simulation.

Table 2-2 summarizes the initialization calculations that are performed for ozone, NO_x and organics. Note that the expression for organics has been written generally for any organic species. The actual number of species included in the simulation will be dictated by the particular choice of chemical mechanism. With regard to the organic compounds, OZIPM-2 is structured to keep track of nonmethane hydrocarbon compounds separately from oxygenated compounds such as formaldehyde, acetaldehyde, etc. The computational procedures, however, are identical for both types of compounds. The carbon fractions and carbon numbers in Table 2-2 (i.e., f_i, $(f_{ts})_i$, $(CN)_i$) must be specified by the user when a mechanism other than DODGE is used, and these will be discussed in later chapters. For the DODGE mechanism, default numbers are preset in OZIPM-2, and the reader is referred to Reference 6 for a discussion of default assumptions. The initialization procedures for ozone and NO_x are the same for both OZIPM-2 and OZIPP, and are not affected by choice of mechanism.

2.1.2 Dilution

In OZIPM-2, dilution occurs as a result of the rise in the mixed layer. As shown in Table 2-1, the dilution rate is determined at any particular time in the simulation by dividing the rate of mixing height rise by the magnitude

TABLE 2-2. DETERMINATION OF INITIAL CONCENTRATIONS

1. Ozone

$$[O_3]_o = [O_3]_{ts}$$

where

$[O_3]_o$ = initial concentration of ozone, ppmV

$[O_3]_{ts}$ = ozone concentration transported in surface layer, ppmV (default is zero)

2. NO_2, NO

$$[NO_2]_o = [NO_x]_o f_{NO2} + [NO_x]_{ts}$$

$$[NO]_o = [NO_x]_o (1-f_{NO2})$$

where

$[NO_2]_o$ = initial concentration of NO_2, ppmV

$[NO]_o$ = initial concentration of NO, ppmV

$[NO_x]_o$ = initial concentration of NO_x, ppmV

f_{NO2} = fraction of initial NO_x that is NO_2 (default = 0.25)

$[NO_x]_{ts}$ = NO_x concentration transported in surface layer, ppmV (default is zero)

3. Organics

$$[HC_i]_o = \left\{[NMOC]_o (f_i) + [NMOC]_{ts} (f_{ts})_i\right\} /(CN)_i$$

where

$[HC_i]_o$ = initial concentration of organic species i, ppmV

$[NMOC]_o$ = initial concentration of total NMOC, ppmC

f_i = fraction of NMOC that is organic species i (ppmC basis)

$[NMOC]_{ts}$ = NMOC concentration transported in surface layer, ppmC

$(f_{ts})_i$ = fraction of surface transported NMOC that is organic species i (ppmC basis)

$(CN)_i$ = number of carbon atoms associated with organic species i (i.e., the carbon number) of the mixing height. Thus, the dilution rate is determined solely by the diurnal profile of the mixing height used in the simulation. Within OZIPM-2, two options exist for specifying this pattern. In the first, the growth in the mixed layer is governed by a generic, preset, characteristic curve.[11] With the second option, the user specifies mixing heights at hourly intervals of the simulation. Each option is discussed in more detail below.

The characteristic curve relates the fraction of growth in mixing height during any particular day to the corresponding fraction of time between sunrise and sunset (see Figure 2-1).* Since the timing of sunrise and sunset varies throughout the year, the OZIPM-2 program internally computes these times for the specific day being modeled. Typically, the user specifies only the mixing height at the start of the simulation and the maximum afternoon mixing height. Alternatively, the user has the option of specifying the time at which the mixing height begins to rise, and the time at which the afternoon mixing height reaches its maximum. In the latter case, the general shape of the characteristic curve will be used, but the timing will conform to the user defined inputs.

As an alternative to the characteristic curve, any particular mixing height profile may be specified by the user. Under this option, the model inputs consist of the mixing heights at each hour of the model simulation. The dilution rate is computed from the specified profile by linear interpolation of the mixing height and the rate of growth between the appropriate hourly inputs. It should be added that the linear interpolation approach introduces discontinuities in

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*This curve has been modified slightly in OZIPM-2 by using cubic-splines to eliminate discontinuities in the dilution rate at inflection points.

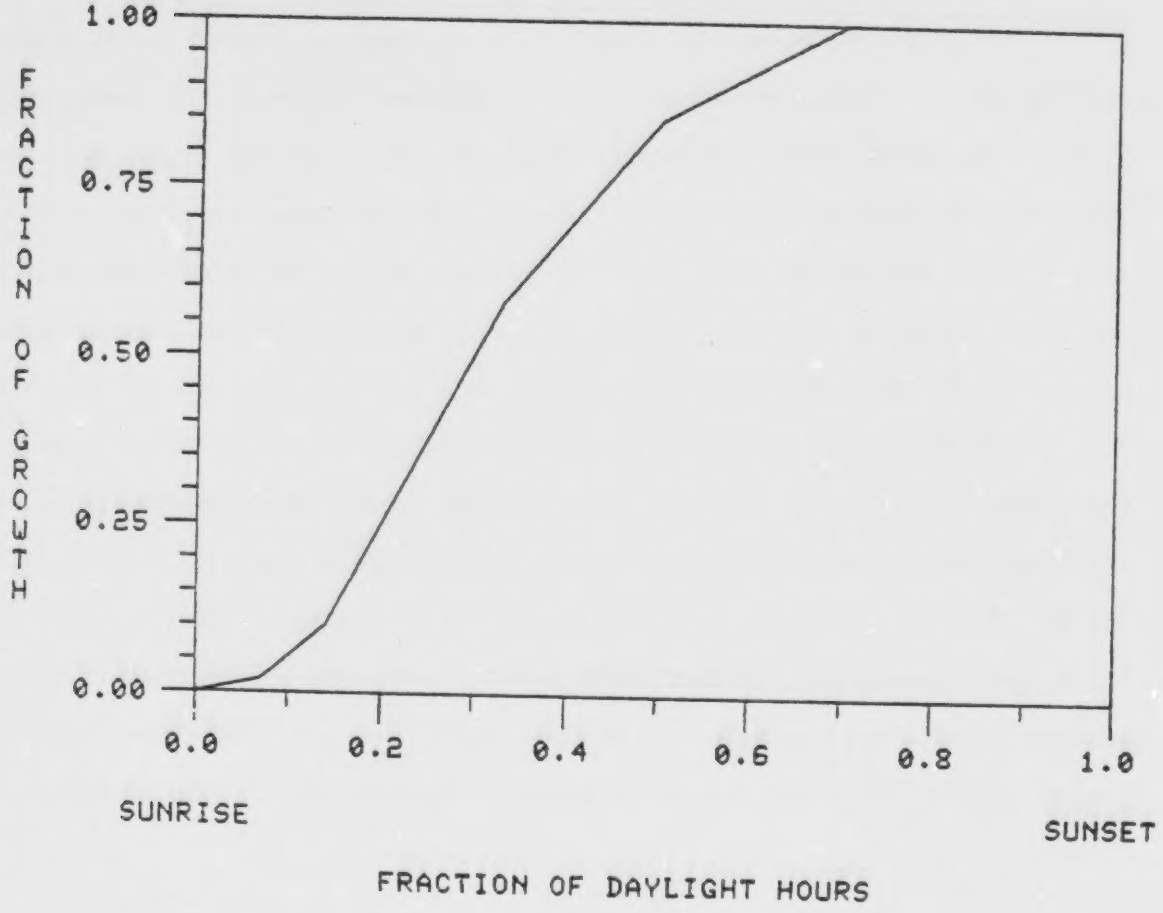


FIGURE 2-1. GRAPHICAL DEPICTION OF CHARACTERISTIC CURVE

the dilution rate due to the abrupt changes in the rate of growth of the mixing height from one hourly interval to the next. Although these discontinuities are not desirable, tests have indicated that their effect on the overall simulation results is not significant.

2.1.3 Entrainment of Pollutants From Aloft

Entrainment is treated essentially the same in OZIPM-2 as in OZIPP. Pollutants from aloft are entrained and distributed uniformly and instantaneously in the mixed layer as a result of growth in the mixing height from its early morning level to its afternoon maximum. The concentrations of the pollutants aloft do not change with time, and thus are assumed to be constant within the layer extending from the top of the mixing height to an altitude at least as high as the afternoon maximum. As shown in Table 2-1, the rate of entrainment of any particular species varies proportionally with the dilution rate and the concentration aloft. Default concentrations of all pollutant levels aloft are zero, but the user may provide inputs for ozone, NO_2 and NMOC. (Note that all NO_x aloft is assumed to be NO_2.) If the concentration of organics aloft is input, and a mechanism other than DODGE is being used, then the user must specify apportioning factors to split total NMOC aloft into the individual organic groups. Table 2-3 gives the mathematical representation of the entrainment process.

2.1.4 Post-0800 Emissions

As in OZIPP, emissions of VOC and NO_x that occur subsequent to the simulation starting time may be included in the model simulations. These emissions are modeled by adding pollutant concentrations to the levels already within the column. The magnitude of the concentration that is added is derived by multiplying a user determined emission fraction times the initial concentration of

TABLE 2-3. MATHEMATICAL REPRESENTATION OF ENTRAINMENT

$$\left.\frac{d[O_3]}{dt}\right|_{ent} = K_D[O_3]_{ta}$$

$$\left.\frac{d[NO_2]}{dt}\right|_{ent} = K_D[NO_x]_{ta}$$

$$\left.\frac{d[HC_i]}{dt}\right|_{ent} = K_D\ (f_{ta})_i[NMOC]_{ta}/(CN)_i$$

where

$\left.\frac{d[O_3]}{dt}\right|_{ent}$, $\left.\frac{d[NO_2]}{dt}\right|_{ent}$, $\left.\frac{d[HC_i]}{dt}\right|_{ent}$ = entrainment rates of ozone, NO_2 and organic species i, ppmV/min

K_D = dilution rate, min^{-1}

$[O_3]_{ta}$, $[NO_x]_{ta}$ = O_3 and NO_x concentrations aloft, ppmV

$[NMOC]_{ta}$ = total NMOC concentration aloft, ppmC

$(f_{ta})_i$ = fraction of aloft NMOC that is organic species i

$(CN)_i$ = carbon number for species i

NMOC or NO_x. (Expressing the emissions as a function of initial concentrations permits easy evaluation of emission changes through manipulation of initial concentrations alone, i.e., hourly emission levels do not have to be adjusted separately.) The emission fractions are expressed on an hourly basis, but the OZIPM-2 model internally converts the hourly data to continuous functions for use in solving the differential equations. In addition to this adjustment, the concentrations added to represent the impact of fresh emissions must be adjusted relative to the column volume. This is done internally within the program by multiplying the concentration times the ratio of the mixing height at the start of the simulation to the height at any particular time in the simulation. The procedures just described are expressed mathematically as shown in Table 2-4. It should be noted that 90% of all NO_x emissions are assumed to be NO, with the remaining 10% being NO_2. Apportionment of total NMOC into individual organic species is accomplished by using the same carbon fractions that are used to apportion initial NMOC concentrations to individual species.

The key inputs to be supplied by the user for post-0800 emissions are the hourly emission fractions. Although they may be specified directly as is done with OZIPP, a special option has been added to OZIPM-2 that allows the user to input information on mass emission rates, initial concentrations, and initial mixing height, and direct OZIPM-2 to compute the emission fractions internally. The procedures used in the computations have been explained in detail in Reference 8, Guideline For Use Of City-specific EKMA In Preparing Ozone SIPs. In summary, an emission fraction may be computed according to the following formula:

TABLE 2-4. MATHEMATICAL REPRESENTATION OF POST-0800 EMISSIONS

$$\left.\frac{d[NO_2]}{dt}\right|_{em} = 0.1\ (E_{NOx})_t\ ({}^{Ho}/{}_{Ht})\ [NO_x]_o$$

$$\left.\frac{d[NO]}{dt}\right|_{em} = 0.9\ (E_{NOx})_t\ ({}^{Ho}/{}_{Ht})\ [NO_x]_o$$

$$\left.\frac{d[HC_i]}{dt}\right|_{em} = f_i\ (E_{NMOC})_t\ ({}^{Ho}/{}_{Ht})\ [NMOC]_o/(CN)_i$$

where

$\left.\frac{d[NO_2}{dt}\right|_{em}$, $\left.\frac{d[NO_2]}{dt}\right|_{em}$, $\left.\frac{d[HC_i]}{dt}\right|_{em}$ = rates of change in concentration due to post-0800 emissions, ppmV/min

$(E_{NOx})_t$, $(E_{NMOC})_t$ = value of emission fractions at time t

H_o = mixing height at start of simulation

H_t = mixing height at time t

$[NO_x]_o$, $[NMOC]_o$ = initial concentrations of NO_x (ppmV) and NMOC (ppmC)

f_i = fraction of total NMOC that is organic species i (same value used for initial conditions)

$(CN)_i$ = carbon number for species i

$$E_i = \frac{Q_i}{\alpha \, CoHo} \qquad (2\text{-}1)$$

where

E_i = emission fraction for hour i

Q_i = mass emission density for hour i, kg/km^2

Co = initial NMOC or NO_x concentration, ppmC or ppm

Ho = mixing height at start of simulation, km

α = conversion factor: 595 kg/km^3 ppmC for organics and 1890 kg/km^3 ppm for NO_x

This new OZIPM-2 option requires the user to specify the initial concentrations of NMOC and NO_x, initial mixing height Ho, and the mass emission density for each hour. (The procedures for formulating these inputs are described in Reference 8 and will not be repeated here.) OZIPM-2 will then compute the hourly emission fractions from this set of information, thereby eliminating the need for the user to compute the fractions manually. When using this option, the model inputs must be expressed in the units indicated in equation 2-1.

2.1.5 Chemical Reaction

The rate of change in pollutant concentration due to chemical reaction is treated identically in OZIPP and OZIPM-2. The overall rate of change is equal to the difference between production rate and rate of loss. The production rate (loss rate) is the sum of all individual rates of reaction in which a species is produced (destroyed). An individual reaction rate is expressed as the product of a concentration term and a reaction rate constant term, e.g.,

$$R_j = k_j \prod_{p=1}^{Nr} C_p \qquad (2\text{-}2)$$

where

R_j = rate of reaction j

k_j = rate constant for reaction j

C_p = concentration of reactant p

Nr = total number of reactants in reaction j

Within OZIPM-2, the DODGE mechanism has been set up in the appropriate format needed for computing the chemical rates of change for each species. When an alternative mechanism is used, the chemical rates of change are derived from the user supplied inputs on the reactants and products of each reaction, and their rate of reaction. Chapter 3 will include a discussion of the specific methods that should be used when encoding a chemical mechanism for use with OZIPM-2.

2.2 DESCRIPTION OF OZIPM-2 OPERATIONS

As described in the introduction to this chapter, the OZIPM-2 user may direct the program to perform three distinct operations:

1. conduct a single simulation,
2. generate an ozone isopleth diagram,
3. calculate a VOC control estimate directly.

The computational procedures used in OZIPM-2 to perform the first two operations are virtually identical to those used in OZIPP, and thus will only be summarized here. For a more complete description of these procedures, the reader is referred to the OZIPP User's Manual, Reference 6.

2.2.1 Single Simulation (CALCULATE)

A single simulation is conducted when the OZIPM-2 user invokes the CALCULATE option. (Chapters 3 and 4 explain in detail the specific inputs associated with the selection of this operation.) In most instances, the user will supply city-specific inputs for the city under review (e.g., city location, date, dilution, post-0800 emissions, transported pollutant levels, etc.). If a mechanism other than DODGE is being used, the user must also supply information on how total NMOC is to be divided into individual organic groups. OZIPM-2 uses this information to set up the differential equations that must be solved (i.e., Table 2-1). In setting up those equations, input variables that vary with time (e.g., dilution rate, post-0800 emissions and photolytic rate constants) are structured so that they may be updated continuously throughout the simulation. The only other set of inputs that must be supplied by the user is the initial concentrations of NO_x and total NMOC. Procedures that may be used to estimate these values are discussed in Section 3.3 of Reference 9, Guideline For Using The Carbon-Bond Mechanism In City-specific EKMA. (Note that, while Reference 9 is directed towards use of the carbon-bond mechanism, the procedures described in that section are applicable to the use of any chemical mechanism with EKMA.)

In performing a single simulation, OZIPM-2 numerically integrates the set of differential equations discussed in the previous sections. Since the numerical integration scheme has been discussed in Reference 6, the OZIPP User's Manual, it will not be repeated here. The solution produces instantaneous concentrations of individual species as a function of time. OZIPM-2 will also compute the maximum one-hour average concentration of a specified pollutant that occurs during the simulation. While this operation is routinely performed for ozone, the user has the option of changing to another pollutant by means of the SPECIES option (discussed in Chapters 3 and 4). The user also has the option of controlling the amount of information about the solution that is displayed. With the default operational mode, concentrations of major pollutants (e. g., NMOC, NO_x and ozone) are shown at hourly intervals (e.g., 0800, 0900, 1000, etc.). However, the user may control the times at which the concentrations are displayed (e.g., half-hour intervals), and may display additional information such as the concentrations of all species in the mechanism, the rates of all chemical reaction, and the overall time rates of change of the species due to both chemical and physical processes. Again, these options will be more fully discussed in subsequent chapters.

2.2.2 Isopleth Diagram (ISOPLETH)

An isopleth diagram is a graphical display of maximum one-hour average concentrations of any pollutant plotted as a function of initial NMOC and NO_x concentrations. An example ozone isopleth diagram is shown in Figure 2-2. Such a diagram is created by performing repeated single simulations in which all variables except the initial NMOC and NO_x concentrations remain unchanged from simulation to simulation. The initial NMOC and NO_x concentrations used in the individual simulations must be chosen in a way that will provide good diagram definition (i.e., provide enough points that are sufficiently well spaced to permit accurate interpolation). The final step involves using the single simulation results to interpolate and plot the isopleths representing specific, one-hour average concentration levels.

The OZIPM-2 procedures for generating an ozone isopleth diagram are the same as those used in OZIPP, and will only be briefly described here. Single simulations are first performed using the initial NMOC and NO_x concentrations corresponding to each of the four corners of the diagram. Two more simulations are performed for the diagram edges in an attempt to locate the intersection points of the lowest valued isopleth with those edges. After performing these six simulations, the initial NMOC and NO_x concentrations for subsequent calculations are chosen along radial lines emanating from the origin (i.e., lines corresponding to constant ratios of NMOC to NO_x). Finally, two simulations are again performed for the diagram edges to aid in the location of the lowest valued isopleth. As with OZIPP, the OZIPM-2 user may control the scales of the abscissa (NMOC) and the ordinate (NO_x), the number of NMOC/NO_x radials used, and the

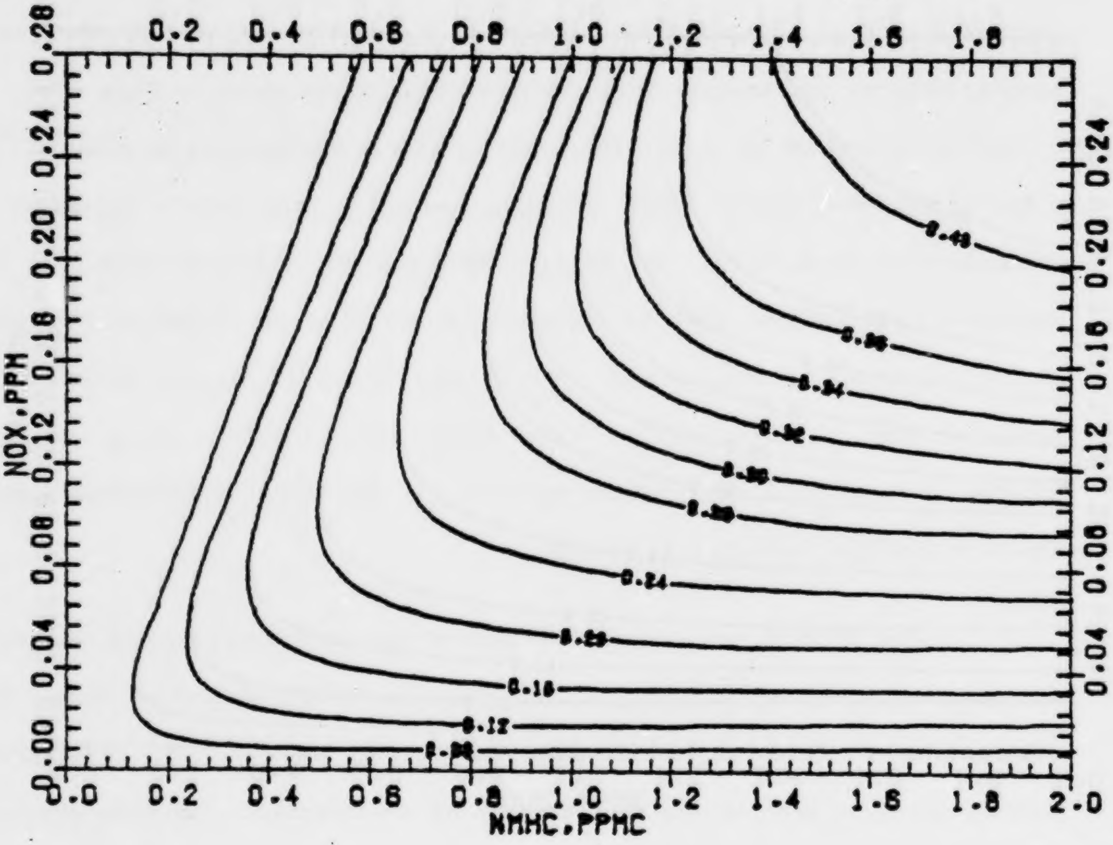


Figure 2-2. Example Ozone Isopleth Diagram

number of points along those radials that are used in the simulations. The selection of the individual simulation points is, however, controlled internally by OZIPM-2.

The selection of the individual simulation points along each radial, and the drawing of a smooth curve of constant concentration through the data points generated from the single simulations are both controlled by an interpolation scheme that makes use of hyperbolic splines. The hyperbolic spline approach was selected over the cubic spline approach since kinetic systems generally yield curves more closely resembling exponential functions. A noteworthy feature of the hyberbolic splines is the existence of a tension factor that affects the interpolated values. The lowest value drives the interpolation towards the cubic-spline approach, while the highest value drives the interpolation towards piece-wise linear interpolation. While the tension factors are adjustable by the user, the default values should be adequate in most cases.

Whenever the ISOPLETH option is invoked, a line-printer diagram is always produced. The OZIPM-2 user also has the option of producing a diagram on an off-line plotter (such as CALCOMP). The only major new feature of OZIPM-2 is the capability to produce an isopleth diagram of any particular species, rather than just ozone. Although the default species is ozone, the user may select any other species by invoking the SPECIES option, which will be discussed in Section 3.2.4.4.

2.2.3 Control Calculation (EKMA)

A major new feature of OZIPM-2 is the capability to compute directly the percent reduction in NMOC needed to lower peak ozone to the level of the ozone NAAQS, i.e., 0.12 ppm. Heretofore, this particular computation has usually been performed using an ozone isopleth diagram. The new feature permits the computation to be done analytically without performing all the simulations needed to generate an ozone isopelth diagram. Since the new procedure is simply an automated method of using an ozone isopleth diagram, the concepts underlying the use of such a diagram to compute VOC control estimates should be fully understood. Detailed discussions have been presented in References 3 and 8, and only the major points will be addressed here. For additional information, the reader may wish to consult these two references.

A control estimate calculation performed with an ozone isopleth diagram begins by establishing a starting point on the diagram. This base-case point is located by finding the intersection of a design NMOC/NO_x ratio line with the isopleth corresponding to the base-case ozone value. Typically, the NMOC/NO_x ratio used in the calculation is derived from 6-9 a.m. measurements of NMOC and NO_x taken in the urban core, and the base-case ozone value corresponds to a peak ozone concentration measured within or downwind of the city under review (see for example, Reference 8). Conceptually, the base point corresponds to existing conditions in the city (i.e., observed ozone, base emissions, base transport levels, etc.). All other points on the diagram represent the effects of changing precursor emissions relative to the base-case, assuming everything else remains constant.

In order to determine how much VOC emissions must be reduced to lower the observed ozone peak to 0.12 ppm, the change in NO_x must be accounted for. Usually, this is done by estimating the change in NO_x emissions expected to occur between the base-case time (say, 1984 for example) and the time at which the ozone standard is to be achieved (e.g., 1987). This information is then incorporated in the EKMA analysis by adjusting the NO_x base-case coordinate by the expected percentage change in NO_x emissions. This new, adjusted NO_x coordinate, referred to as the post-control NO_x coordinate, is thus calculated as follows:

$$(NO_x)_2 = (NO_x)_1 \times (1 - \frac{\Delta NO_x}{100}) \qquad (2\text{-}3)$$

where

$(NO_x)_2$ = post-control NO_x coordinate, ppm

$(NO_x)_1$ = base NO_x coordinate, ppm

(ΔNO_x) = anticipated percentage change in NO_x emissions

The corresponding NMOC post-control point is found by locating the intersection of the NO_x post-control point, $(NO_x)_2$, with the 0.12 ppm ozone isopleth. The VOC reduction estimate is then obtained by computing the percentage change between the NMOC base coordinate and the post-control coordinate, or

$$\text{percent reduction} = [1- \frac{(NMOC)_2}{(NMOC)_1}] \times 100 \qquad (2\text{-}4)$$

An example problem illustrating these concepts is shown in Figure 2-3.

The basis for the direct control calculation feature in OZIPM-2 (i.e., the EKMA routine) lies in the fact that the base-case point and the post-control point correspond to single simulations. For the base-case point, the NMOC and NO_x coordinates represent the initial concentrations, in the specified ratio, that generate the base-case ozone concentration. For the post-control point, the NMOC coordinate corresponds to the initial NMOC concentration that generates 0.12 ppm ozone, given the post-control NO_x coordinate. The EKMA routine conducts single simulations within an iterative search procedure to locate these two points, and then calculates the percent change between the base and post-control NMOC coordinates (i.e., $[NMOC]_1$ and $[NMOC]_2$).

GIVEN: O_3 Daily Design Value = .24

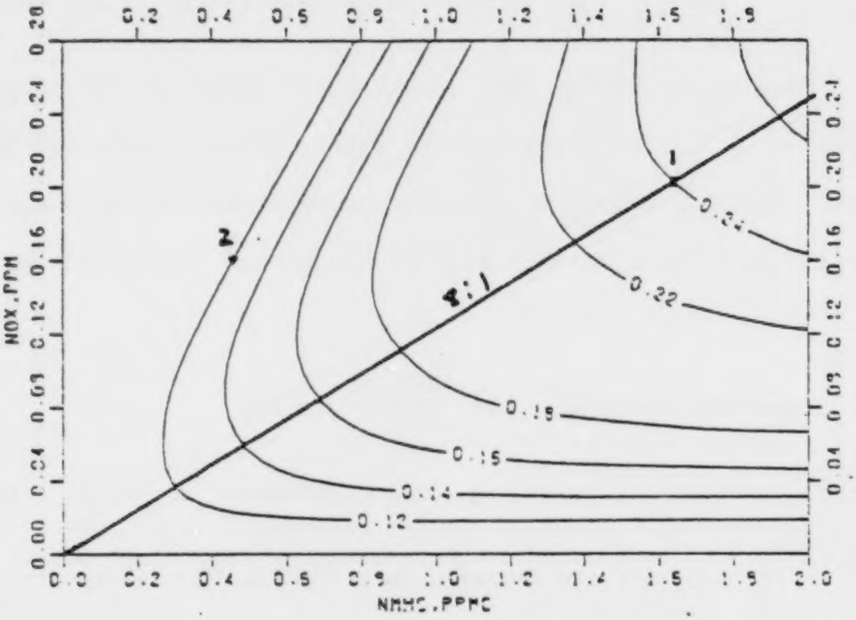
Design NMOC/NO_x = 8:1

Anticipated Change in NO_x = -20%

Base case diagram shown below

FIND: Percent reduction in VOC emissions needed to reduce ozone from .24 to 0.12 ppm

SOLUTION:



STEP 1: The base case point is found by the intersection of the 8:1 NMOC/NO_x ratio line with the .24 ozone isopleth (Point 1) on the diagram. At Point 1, $(NMOC)_1 = 1.64$ and $(NO_x)_1 = .205$

STEP 2: The post-control NO_x coordinate is calcualted as follows:

$$(NO_x)_2 = (.205) \times (1 - \frac{20}{100}) = .164$$

STEP 3: The post-control point is located at the intersection of the .164 NO_x coordinate and the 0.12 ppm ozone isopleth (Point 2). At Point 2, $(NMOC)_2 = 0.46$

STEP 4: The VOC emission reduction is calculated as

$$\% \text{ reduction} = (1 - \frac{.46}{1.64}) \times 100 = 72\%$$

Figure 2-3. Example emission reduction calculation using a single ozone isopleth diagram

The iterative search procedure employed in OZIPM-2 is a modified form of that developed by the Missouri Department of Natural Resources for use with OZIPP.[13] With this procedure, the user must supply the design NMOC/NO_x ratio and the base-case ozone value. OZIPM-2 then searches for the initial NMOC and NO_x coordinates that generate a maximum ozone concentration within 0.0005 ppm of the desired value (i.e., the base-case ozone concentration for the starting point, or 0.12 ppm for the post-control point). In conducting the search, the number of simulations performed is limited to ten. If a solution has not been found within this limit, the program exits from the EKMA routine with a message to that effect. Should this situation occur, the user is advised to generate an isopleth diagram and perform the control calculations graphically. If a solution cannot be obtained with an isopleth diagram either, the user should check all model inputs to insure that they have been correctly specified.

OZIPM-2 begins the search for the starting point by conducting a simulation with the initial NMOC concentration set to 1.0 ppmC, and the initial NO_x concentration equal to 1.0 ppmC divided by the input design NMOC/NO_x ratio. A second simulation is then performed with an NMOC initial concentration that is computed as the product of 1.0 ppmC and the ratio of input base-case ozone value to the maximum ozone concentration found from the first simulation. (The NO_x initial concentration is also updated by dividing the second NMOC estimation by the design NMOC/NO_x ratio.) All successive approximations are then based on the results of the previous two, according to the following linear interpolation scheme.

$$(\mathrm{NMOC})_{I+1} = (\mathrm{NMOC})_I + \frac{(O_3)_B - (O_3)_I}{(O_3)_I - (O_3)_{I-1}} \times [(\mathrm{NMOC})_I - (\mathrm{NMOC})_{I-1}] \quad , (2\text{-}5)$$

where I refers to the iteration number, (NMOC) refers to the NMOC initial concentration used in the simulation, (O_3) to the maximum ozone concentration computed in the simulations, and $(O_3)_B$ to the base-case ozone value. As with the first two simulations, the NO_x initial concentration is always computed by dividing the NMOC initial concentration used in this simulation by the input design NMOC/NO_x ratio. In the event an approximation of the NMOC initial concentration should be negative, it is reset to 0.1 ppmC.

The search routine for the post-control point is virtually identical to that used to find the base case point. In this procedure, however, repeated simulations are performed until the predicted ozone concentration is within 0.0005 ppm of 0.12 ppm. Although the initial NMOC concentrations used in successive simulations are computed according to equation 2-5, the NO_x coordinate always corresponds to the post-control NO_x coordinate computed according to equation 2-3. Also, when determining the post-control point, the OZIPM-2 program has the capability of considering changes in precursor transport levels that could occur. The user has the option, therefore, to change the levels of transport to conditions indicative of the post-control state. Conceptually, this is similar to using two isopleth diagrams as has been discussed in Reference 8, Guideline For The Use Of City-specific EKMA In Preparing Ozone SIPs. The reader is referred to this document for methods which can be used to estimate the post-control transport values.

As is readily apparent from the discussions above, use of the EKMA routine bypasses the need to generate an ozone isopleth diagram for most control calculations. As noted above, however, situations may arise in which the iterative search procedure fails to find a solution. In these situations, the user may wish to fall back to the isopleth diagram approach for performing the needed calculations. Furthermore, the EKMA routine focuses on two single simulations, i.e., the base-case point and the post-control point, corresponding to an ozone peak of 0.12 ppm. An ozone isopleth diagram displays graphically ozone changes relative to changes in precursor levels over a wider range and for a continuous range of NMOC/NO_x ratios. Thus, the generation of an ozone isopleth diagram will typically provide more information than the EKMA routine, and may be a preferable approach in some situations.

3.0 OZIPM-2 OPTIONS AND DATA REQUIREMENTS

The operational structure of OZIPM-2 is virtually identical to that of OZIPP. The program contains preset default values that can be used to generate the so-called Standard Ozone Isopleth Diagram (see Reference 3). In most instances, however, the OZIPM-2 user will desire to incorporate city-specific information on dilution, light intensity, post-0800 emissions, etc., and perhaps use a chemical mechanism other than the one embedded in the program (i. e., the DODGE mechanism). Inputs such as these are controlled by selecting one or more specific program options for each type of input. Further, the user controls the functional mode of program operation by selecting one of three major options: (1) the CALCULATE option to perform a single simulation, (2) the ISOPLETH option to generate an isopleth diagram, or (3) the EKMA option to perform a single VOC control calculation. All of the options available to the user are discussed in this chapter, along with their individual data requirements. Information on the specific formats that are used to code the data for input to OZIPM-2 is contained in the next chapter, the User's Guide.

3.1 OVERVIEW OF OZIPM-2 OPERATION

Inputs are supplied to OZIPM-2 by means of input records that are identified by special option code words. Even though OZIPM-2 contains several new options, most of the options are identical to those contained in OZIPP, and these are summarized in Table 3-1. The new options that have been incorporated in OZIPM-2 are summarized in Table 3-2.

To activate any of the options described in Tables 3-1 or 3-2, the input data must contain an input record with the appropriate code word beginning in column 1. Only the first four characters of any code word need be specified, and these will be underlined throughout the remaining text. Associated with

TABLE 3-1. OPTIONS COMMON TO BOTH OZIPP AND OZIPM-2

° ISOPLETH - This option calls for an isopleth diagram to be constructed according to all specified input parameters. The parameters associated with this option include specification of the maximum NMOC and NO_x concentrations to be considered, and selection of the isopleth levels to be drawn. Default values are as follows: maximum NMOC is 2.0 ppmC; maximum NO_x is 0.28 ppm; and 11 concentration levels to be plotted, 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36, and 0.40 ppm. An additional parameter activates printing solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation. This information will not be printed under default conditions.

° CALCULATE - With this option, only one simulation is performed (i.e., only one diagram point calculated) according to the specified input parameters. No isopleth diagram is produced. Initial NMOC and NO_x concentrations must be input with this option. An additional parameter activates the printing of the following: reaction rates, species concentrations, net rates of change in concentrations of all species, and photolytic rate constants for user specified times during the simulation. This information will not be printed under default conditions.

° PLOT - This option activates the drawing of the isopleth diagram on an offline plotter. Standard CALCOMP routines are used. Input parameters associated with this option control the physical dimensions of the offline plot. Parameters to be specified and their associated default values are as follows: length of abscissa (8.5 inches), length of ordinate (5.95 inches), character and number size (0.10 inches), and label size (0.07 inches). An additional parameter activates the overlaying of a grid of different color on the diagram. Under default conditions, the grid is not drawn.

° TITLE - This option allows the user to title the program output. Under default conditions, all output is titled "Standard Ozone Isopleth Conditions."

° PLACE - This option allows determination of the photolysis constants in the kinetic mechanism according to geographical location and time of year. Input parameters associated with this option include the geographic location of the urban area (latitude and longitude), the time zone in which the urban area is located and the time of the simulation. Default values are for a simulation for Los Angeles, California, on June 21, 1975.

° REACTIVITY - This option allows the user to specify reactivity factors for the chemical mechanism. For the DODGE mechanism, these are the fraction of NMOC that is propylene and the fraction of NMOC to be added as aldehydes. (Default values for these parameters are 0.25, and 0.05, respectively.) For other mechanisms, the user must supply inputs on organic reactivity. These option also allows the user to specify initial NO_2/NO_x ratio, whose default value is 0.25.

TABLE 3-1. OPTIONS COMMON TO BOTH OZIPP AND OZIPM-2 (continued)

° EMISSIONS - This option permits the consideration of post-0800 emissions. Under default conditions, post-0800 emissions are assumed zero. To override this assumption, the user must specify the fractions of the initial NMOC and/or NO_x concentrations that are to be added each hour to represent the effect of post-0800 emissions. This option is not used if the MASSEMISS option described in Table 3-2 is invoked.

° TRANSPORT - This option allows the consideration of transported pollutants. Pollutants can be transported in both the surface layer and aloft. Input parameters include the initial surface layer transported concentrations of NMOC, NO_x and ozone, and the concentrations of these pollutants in the air above the mixed layer. All of these concentrations are assumed zero under default conditions.

° DILUTION - This option allows for the consideration of dilution due to the rise of the mixing height. Input parameters include the height of the mixed layer in the morning, the final height after the rise, the time at which the rise begins, and the time at which it reaches its final height. Under default conditions, the mixed layer is assumed to rise from 510 meters at 0800 LDT to 630 meters at 1500 LDT.

° ALREADY - This option permits the use of results from a previous simulation. Input parameters include the initial NMOC concentration, the initial NO_x concentration and the maximum one-hour ozone concentration from each previous simulation. Under default conditions, this option is not exercised.

° ACCURACY - This option controls the number of simulations, the accuracy of each simulation and the accuracy of the interpolations. Input parameters and their associated default values are as follows: the number of constant NMOC/NO_x radials to be included in the simulations (11), the number of simulations per radial line (5), the error tolerance in the numerical integration scheme (0.01), the tension factor for the first stage of interpolation (1.0), and the tension factor for the hyperbolic spline functions used in plotting isopleths (1.0).

TABLE 3.2. NEW OZIPM-2 OPTIONS

° MECHANISM - This option provides for the use of a chemical mechanism other than the default DODGE mechanism. Inputs required include reactants, products, rate constants, and activation energies (optional) for each reaction, and identification of the organic species and photolytic reactions.

° TIME - This option permits the user to control the simulation times. Default starting and ending times are 0800 LDT and 1800 LDT, respectively.

° MIXING - This option permits the user to specify mixing heights at hourly intervals.

° SPECIES - This option permits the user to calculate maximum one-hour average concentrations and construct isopleth diagrams for any species contained in the chemical mechanism.

° MASSEMISS - This option allows the user to specify post-0800 emissions on a mass-density basis (i.e., kg/km^2), and direct OZIPM-2 to compute post-0800 emission fractions.

° INITIAL - This option permits the user to specify initial concentrations of species other than the organic compounds, NO_x and ozone.

° EKMA - This option directs the OZIPM-2 program to perform a control reduction calculation with user specified input ozone design value and $NMOC/NO_x$ ratio.

any input record containing an option code word are six numeric fields, each 10 columns wide, beginning in column 11. Any numerical data that may be required by a particular option are coded in these fields, and any additional data that may be required are supplied in input records that immediately follow the option record. With the exception of the MECHANISM option, all numerical data that may be required in subsequent input records are supplied in records made up of seven fields that are 10 columns wide and begin in column 1. Alphanumeric information that may be needed is supplied in a subsequent input record beginning with the first column. It should also be added that the input information required by a particular option may be affected by the selection of other options. For example, a single input record for the REACTIVITY option is needed when the default mechanism is being used, but more than one input record may be required when an alternate mechanism is being used. Finally, most numeric data associated with any particular option have preset default values. In these cases, the preset default value will be used whenever a numeric field is left blank.

The OZIPM-2 program is structured to process the input option records in a sequential manner, and with a few exceptions, the order of the input records is not critical. The first exception is that multiple input records required by any particular option must be grouped together in the proper order (i.e., input option with the code word first, followed by the records containing the required data). Second, all options used to provide city-specific or other inputs (e.g., MECHANISM) must be placed before one of the options that controls the program operation (i.e., CALCULATE, ISOPLETH or EKMA). If any particular input is not provided by the user before one of these options is read by the program, then the pre-set default values will be used. For example, if the MECHANISM option is not used to provide an alternate chemical mechanism, then the default mechanism will be used in the simulations performed by the program.

Additional information on the organization of the input records is contained in the last section of this chapter, and examples are included in Chapter 5.

3.2 DESCRIPTION OF OZIPM-2 OPTIONS

For purposes of the ensuing discussion, the OZIPM-2 options have been grouped according to the following general categories:

- Alternative Mechanism Inputs
  - MECHANISM
- City-specific Inputs
  - PLACE
  - DILUTION
  - MIXING
  - REACTIVITY
  - EMISSIONS
  - MASSEMISS
  - TRANSPORT
- Program Operation Control
  - CALCULATE
  - ISOPLETH
  - EKMA
- Additional Simulation Options
  - TITLE
  - PLOT
  - TIME
  - SPECIES
  - INITIAL
  - ACCURACY
  - ALREADY

Although each of the options listed above will be discussed, most emphasis is placed on describing the new OZIPM-2 options. The user may wish to refer to Reference 6, the OZIPP User's Manual, for additional details regarding the options common to both OZIPP and OZIPM-2.

3.2.1 Alternative Mechanism Inputs (MECHANISM)

A major feature of the OZIPM-2 program is the capability to accept as an input a chemical mechanism other than the default DODGE mechanism. Since chemical kinetic mechanisms are typically lengthy, a substantial amount of information is usually required for input. Also, the incorporation of a chemical mechanism in any photochemical model can be a complicated procedure. Since each mechanism's characteristics and structure are unique, only general guidance on developing mechanism inputs can be provided here. In the event that guidelines are not available on incorporating a specific mechanism in OZIPM-2 (e.g., Reference 9 on using the Carbon-bond mechanism), the user is advised to consult with a photochemical modeling specialist familiar with both OZIPM-2 and the mechanism of interest.

As noted earlier, chemical mechanism inputs are supplied to OZIPM-2 by means of the MECHANISM option. These inputs must include the individual chemical reactions (i.e., reactants and products of each reaction) and the rate constants for all non-photolytic reactions. The user must also identify all photolytic reactions, specify how the diurnally varying photolytic rates of reaction are to be determined, identify all organic species, and specify their respective carbon numbers (i.e., the number of carbon atoms associated with each organic group.) In addition, the user has the option of providing activation energies for individual reactions, and specifying the temperature used to determine individual rate constants. Before describing the specific mechanism inputs that are needed for OZIPM-2, some general concepts associated with developing these inputs for any particular mechanism are discussed below.

3.2.1.1 Mechanism Structure.

A chemical kinetic mechanism consists of a group of individual chemical reactions and their associated rates of reaction. In general, the OZIPM-2 inputs include the reactants and products of each reaction, and the rate at which the reaction proceeds (i.e., the rate constant). However, the structure of the mechanism must conform to the format required by OZIPM-2. The discussion below begins with a description of how the individual reactions must be structured for input to OZIPM-2, and how some reactions may be transformed to the required form.

Structure of Individual Reactions. Each species in the mechanism must be identified consistently throughout the mechanism by a unique, alphanumeric code (up to four letters). Except for species that photolyze, the selection of the species code is entirely up to the user. (As an example, the species NO_3 and HNO_3 might be represented by NO3 and HNO3, respectively.) The total number of reactions that may be input is limited to 200, and the total number of mechanism species is limited to 80. In addition, the user must assign a unique identification number to each reaction, although these need not be numbered sequentially. For each reaction, the total number of reactants is constrained to three, and the total number of products to four. Further, the stoichiometric coefficients of each reactant and product must be one. Thus, for example, a reaction of the form

$$A + B \dashrightarrow 2C \qquad (3\text{-}1)$$

would have to be rewritten as

$$A + B \dashrightarrow C + C \qquad (3\text{-}2)$$

Some additional guidelines for restructuring individual reactions to conform to the appropriate form for input to OZIPM-2 are contained in Appendix B.

Rate Constants. For each non-photolytic reaction, the rate constant at 298°K must be specified. The user may also specify activation energies (in °K) for each reaction. If so done, the rate constant is computed at the simulation temperature (default = 303°K) according to Arrhenius's Law, i.e.,

$$k_T = k_{298}\, e^{\Delta E\left(\frac{1}{298} - \frac{1}{T}\right)} \qquad (3\text{-}3)$$

where

k_T = reaction rate constant at temperature T

k_{298} = input rate constant at 298°K

ΔE = input activation energy, °K

Finally, it should be added that reactions in which some of the reactant concentrations do not vary with time (e.g., oxygen) may be transformed to lower order reactions by using a psuedo rate constant that is the product of the true reaction rate constant and the concentration of the invariant species. The reader is referred to Appendix B for a more detailed discussion.

Photolytic Reactions. The proper selection of photolytic reaction rates depends to a large extent on the structure of the chemical mechanism under consideration. As a consequence, specific guidance cannot be provided here. The discussion that follows focuses on describing the various options that are available to the OZIPM-2 user in dealing with photolytic reactions. Since photolytic reactions are among the most important in any chemical mechanism, their proper treatment is essential. As suggested earlier, consultation with a photochemical modeling specialist is advised when specific guidance is unavailable.

The OZIPM-2 program internally generates photolytic reaction rates for nitrogen dioxide, ozone, nitrous acid, hydrogen peroxide, formaldehyde, and acetaldehyde using the computer code developed by Schere and Demerjian.[13] These rates correspond to zero cloud cover conditions, and are for reactions at the earth's surface. The photolysis rates for the individual species are made city-specific by means of the PLACE option that makes use of the date and city location to determine the individual rates. (The PLACE option will be discussed in a subsequent section.)

In OZIPM-2, the maximum number of photolytic reactions permitted is eight, and the species that photolyze must be identified by one of the following pre-defined codes:

NO2 = nitrogen dioxide
O3 = ozone
HONO = nitrous acid
H2O2 = hydrogen peroxide
HCHO = formaldehyde
ALD2 = acetaldehyde

For ozone and formaldehyde, two separate photolytic pathways are possible:

$$\text{HCHO} \xrightarrow{h\nu} \text{stable products} \qquad (3\text{-}4)$$

$$\text{HCHO} \xrightarrow{h\nu} \text{radical products} \qquad (3\text{-}5)$$

$$O_3 \xrightarrow{h\nu} O(^1D) + O_2 \qquad (3\text{-}6)$$

$$O_3 \xrightarrow{hv} O(^3P) + O_2 \qquad (3\text{-}7)$$

If the mechanism contains photolytic reactions for either HCHO or O_3, then both pathways must be included in the mechanism. Thus, for example, it is not permissible to have HCHO photolyzing to just radical products.

In addition to the special code words defined above, the user assigned identification number of each photolytic reaction must be specified, and "rate constants" for each photolytic reaction must also be supplied. These "rate constants" are actually multiplicative constants used to adjust the rate constants generated internally by OZIPM-2, i.e.,

$$K_{actual} = (K_{input})(K_{OZIPM\text{-}2}) \qquad (3\text{-}8)$$

where

K_{actual} = photolytic rate used in the simulation

K_{input} = multiplicative constant input by user

$K_{OZIPM\text{-}2}$ = photolytic rate generated internally by OZIPM-2

In Equation 3-8, $K_{OZIPM\text{-}2}$ corresponds to the photolytic rates generated for NO_2, O_3, HONO, H_2O_2, HCHO, or ALD2, with the appropriate value determined by the selected species code-word (i.e. K_{NO_2}, K_{O_3}, K_{HONO}, etc.) If the rates to be used in the model simulations are to be identical to those generated by OZIPM-2, the input photolytic "rate constants" (i.e., the multiplicative constants) should be set to 1.0. Again, the choice of the multiplicative constant will generally be dictated by the structure of the mechanism. Note, however, that updates to theoretical photolysis rates can be handled at least partially by the multiplicative constants as well.*

---

*Updates to photolytic rates may lead to different patterns that are not directly proportional to the older rates over the entire diurnal cycle. In such cases, the multiplicative constants can only be used to approximate the updated patterns.

In some chemical mechanisms, photolytic reaction rates may be expressed relative to the photolytic reaction rate of NO_2. For example, in the CB-3 mechanism, the photolytic reaction for the ALD2 species is equal to 0.02 times the rate of NO_2 photolysis. To handle situations such as this, the multiplicative constants are input as usual, (e.g., .02 in this example), but the reactions of this form must be specifically identified by the user-defined reaction identification number. In the example, the identification of the reaction number for ALD2 photolysis directs the program to use K_{NO_2} instead of K_{ALD_2} in equation 3-8 to determine the ALD2 photolysis rate.

Organic Species. A key component of any chemical mechanism is the treatment of organic species. Because the total concentration of organic species must be apportioned to the individual organic groups, those groups must be explicitly identified. Furthermore, the number of carbon atoms associated with each group (i.e., the carbon number) must also be specified. In OZIPM-2, two different classes of organic groups may be used: "hydrocarbons" and "aldehydes." Up to ten "hydrocarbon" species and four "aldehyde" species are permitted. It should be added that it is not necessary to use both classes of organics.* For example, the organic species normally thought of as aldehydes could be included in the "hydrocarbon" class, thereby eliminating the need to provide separate inputs for both the hydrocarbons and aldehydes. Whichever convention is ultimately used, the apportioning scheme must be accurately specified. (This will be discussed further in Section 3.2.2). If the convention is adopted whereby aldehydes are not explicitly named in the mechanism (i.e., the mechanism aldehyde species are included with the hydrocarbon class), a message will be printed to that effect. This message can be ignored, provided aldehydes have been properly accounted for in the mechanism.

---

*It should be emphasized that chemical mechanisms always contain both hydrocarbon and aldehyde species. What is meant here is that it is not always necessary to use the OZIPM-2 naming conventions to account for each.

3.2.1.2 MECHANISM Inputs

The inputs to OZIPM-2 that are are supplied by means of the MECHANISM option can be quite lengthy. To facilitate the discussions that follow, a sample set of inputs is shown in Table 3-3.* The first column of each input record corresponds to the location of M in the first input record. The sequential numbers to the extreme left refer to the input record number. Thus, there are 87 input records associated with this particular mechanism. Finally, in the ensuing discussions, reference will be made to the reaction identification numbers. These numbers are located in the middle portion of the input records, beginning with record number six.

The mechanism option code word (i.e., MECH) is located in columns 1-4 of the first input record (see Table 3-3). Additional numerical data required by this option are located in the six numeric fields beginning in column 11. (Recall that each field is ten columns wide, so the starting locations for these fields are columns 11, 21, 31, 41, etc.). The first numeric field must contain the identification number of the last reaction in the mechanism. In the example shown in Table 3-3, the last reaction identification number is 99. The second field contains the total number of photolytic reactions in the mechanism (i.e., seven in the example). The total number of hydrocarbon species is entered in the third field, and the total number of aldehydes is entered in the fourth field. In the example shown in Table 3-3, seven hydrocarbon species are indicated, and since the fourth field was left blank, aldehyde species are not

---

*The mechanism shown in Table 3-3 is the CB-3 mechanism discussed in References 9 and 14.

Table 3-3. CB-3 Mechanism Inputs for OZIPM-2.

```
 1   MECH        99.        7.0          7.0                                   1.0
 2   1.          71.        99.          73.         38.         37.           67.
 3   67.
 4   PAR         ETH        OLE          ARO         HCHO        ALD2          NR
 5   1.          2.         2.           6.          1.          3.            1.
 6   NO2                 1       NO          O                                 1.00E+0
 7   O                   2       O3                                            4.40E+6
 8   O3    NO            3       NO2                                           2.66E+1  1450.0
 9   O3    NO2           4       NO3                                            4.8E-2  2450.0
10   O     NO2           5       NO                                            1.30E+4
11   O3    OH            6       HO2                                            1.0E+2  1000.
12   O3    HO2           7       OH                                             2.4E+0  1525.0
13   NO2   OH            8                                                      1.6E+4
14   CO    OH            9       HO2                                            4.4E+2
15   NO    NO           10       NO2         NO2                               1.50E-4
16   NO3   NO           11       NO2         NO2                                2.8E+4
17   NO3   NO2          12                                                      2.6E+1  -10600.
18   HO2   NO           13       NO2         OH                                 1.2E+4
19   HO2   HO2          14                                                      1.5E+4
20   PAR   X            15                                                      1.0E+5
21   PAR   OH           16       MEO2                                           1.2E+3  560.0
22   OLE   O            17       MEO2        ACO3        X                      2.7E+3  325.0
23   OLE   O            18       HCHO        PAR                                2.7E+3  325.0
24   OLE   OH           19       RAO2                                           3.7E+4  -540.0
25   OLE   O3           20       HCHO        CRIG                               8.0E-3  1900.0
26   OLE   O3           21       HCHO        MCRG        X                      8.0E-3  1900.0
27   ETH   O            22       MEO2        HO2         CO                     6.0E+2  800.0
28   ETH   O            23       HCHO        PAR                                6.0E+2  800.0
29   ETH   OH           24       REO2                                           1.2E+4  -382.0
30   ETH   O3           25       HCHO        CRIG                               2.4E-3  2560.0
31   ACO3  NO           26       NO2         MEO2                              1.04E+4
32   REO2  NO           27       NO2         HO2         HCHO        HCHO       1.2E+4
33   RAO2  NO           28       NO2         HO2         HCHO        HCHO       1.2E+4
34   MEO2  NO           29       NO2         MEO2        HCHO        X         3.70E+3
35   MEO2  NO           30       NO2         HCHO        HO2                   7.40E+3
36   MEO2  NO           31                                                      9.0E+2
37   REO2  O3           32       HCHO        HCHO        HO2                    5.0E+0
38   RAO2  O3           33       HCHO        HCHO        HO2                    2.0E+1
39   OH    HCHO         34       CRO2        X                                  1.0E+2
40   HCHO  OH           35       HO2         CO                                 9.0E+3
41   HCHO  OH           36       X           ACO3                               8.2E+3
42   HCHO               37       CO                                             2.4E-1
43   HCHO               38       QQ                                            5.64E-1
44   QQ                 81       HO2         HO2         CO                   8.867E+3
45   QQ                 82       MEO2        MEO2        X           XCO      1.133E+3
46   XCO                83       X           CO                                 1.0E+4
47   ACO3  NO2          39       PAN                                            7.0E+3
48   PAN                40       ACO3        NO2                                2.2E-2  13500.0
49   ACO3  HO2          41                                                      1.5E+4
50   MEO2  HO2          42                                                      9.0E+3
51   CRIG  NO           43       NO2         HCHO                               1.2E+4
52   CRIG  NO2          44       NO3         HCHO                               8.0E+3
53   CRIG  HCHO         45                                                      2.0E+3
54   MCRG  NO           46       NO2         HCHO        PAR                    1.2E+4
55   MCRG  NO2          47       NO3         HCHO        PAR                    8.0E+3
56   MCRG  HCHO         48                                                      2.0E+3
```

Table 3-3. CB-3 Mechanism Inputs for OZIPM-2. (continued)

```
57      CRIG
                          49     CO
58      CRIG
                          50                                            6.7E+2
59      CRIG
                          51     HO2     HO2     CO                     2.4E+2
60      MCRG
                          52                                            9.0E+1
61      MCRG
                          53     MEO2    OH      CO                     1.5E+2
62      MCRG
                          54     MEO2    HO2                            3.4E+2
63      MCRG
                          55     HCHO    HO2     HO2     CO            4.25E+2
64      ARO    OH
                          56     RARO                                   8.5E+1
65      ARO    OH
                          57     HO2     OPEN                           6.0E+3 600.0
66      RARO   NO
                          58     NO2     PHEN    HO2                   1.45E+4 400.0
67      OPEN   NO
                          59     NO2     ALD2    X       APRC           4.0E+3
68      APRC
                          60     ALD2    HCHO    CO      X              6.0E+3
69      APRC
                          61     HCHO    HCHO    CO      CO             1.0E+4
70      PHEN   NO3
                          62     PHO     HNO3                           1.0E+4
71      PHO    NO2
                          63                                            5.0E+3
72      PHO    HO2
                          64     PHEN                                   4.0E+3
73      OPEN   O3
                          65     ALD2    X       APRC                   5.0E+4
74      OH     PHEN
                          66     HO2     APRC    PAR     HCHO           4.0E+1
75      ALD2
                          67     HO2     ACO3    CO                     3.0E+4
76      PHEN   OH
                          68     PHO                                    2.0E-2
77      CRO2   NO
                          69     NO2     HCHO    ACO3    X              1.0E+4
78      ALD2   OH
                          70     ACO3    CO                             1.2E+4
79      HONO
                          71     OH      NO                             2.5E+4
80      OH     NO
                          72     HONO                                   3.1E0
81      O3
                          73     O1D                                   9.77E+3
82      O1D
                          74     O                                      5.4E-1
83      O1D
                          75     OH      OH                           4.44E+10
84      OH
                          90     HO2                                    6.8E+9
85      OH
                          91     MEO2                                   8.8E+1
86      NR
                          92     NR                                     2.8E+1
87      O3
                          99     O                                      1.0E+0
                                                                        1.0E+0
```

explicitly identified as such (i.e., they have been grouped with the hydrocarbon species). The fifth field contains the temperature at which the rate constants are computed. In the example, this field is also left blank, indicating that the default temperature of 303°k is to be used. Finally, the last field contains the total number of photolytic reactions whose rates are to be expressed as a function of the NO_2 photolysis rate. (The NO_2 photolysis rate itself need not be included in this number.) For the example, the total number of reactions of this type is 1.

The second input record contains the user defined identification numbers of the photolytic reactions. These entries are located in seven numeric fields, each 10 columns wide, beginning in column 1. If eight photolytic reactions are used, one additional input record would be required (immediately following the second input record), and the identification number of the eighth reaction would be placed in its first numeric field (i.e., columns 1-10). With one exception, the order of the entries in input record two (and three if needed) is not important. The identification numbers for the two HCHO pathways and for the two O_3 pathways must be placed in consecutive fields, respectively. For HCHO, the first entry in the two consecutive fields must be the identification number of the HCHO reaction leading to radical products, and the second entry must be the identification number of the reaction leading to the formation of stable products. For O_3 photolysis, the first entry corresponds to the formation of $O(^3P)$, and the second to $O(^1D)$. Note that in the example, reaction identification number 38 corresponds to HCHO photolysis to radical products, and reaction 37 to photolysis to stable products.

The next input record (number three in the example) contains the user-defined identification numbers for all photolytic reactions whose rate is expressed relative to the NO_2 photolysis rate. In the example, only reaction number 67 is so identified.

The next group of input records contain information on the names of the organic species and their respective carbon numbers. The first record of this set contains the user-defined names of the hydrocarbon species. These are located in the seven fields beginning in columns 1, 11, 21, 31, etc. Again, up to four characters may be used, and the codes must be consistent throughout the mechanism. Since only the first four characters of any field are read, the species names must begin in the exact starting location of each field. (If more than seven hydrocarbon species are used in a mechanism, then the names would be continued on the next input record which would have the exact same format as the first.) Note that in the example, input record number 4 contains the hydrocarbon code names PAR, ETH, OLE, etc. The input record immediately following this one contains the carbon numbers for each hydrocarbon species. The order that these values are entered must correspond exactly to the order in which the hydrocarbon names are entered. Thus, in the example, the carbon number for PAR is 1, the number for ETH is 2, and so forth. (For more than seven hydrocarbon species, carbon number entries would be continued on an input record immediately following the record containing the first seven carbon numbers.) If aldehyde species are to be explicitly named in the mechanism, the next two records would contain the analogous information for them (i.e., one input record with the aldehyde names, followed by another record with the aldehyde species carbon numbers). In the example of Table 3-3, these two records are omitted, since aldehyde species are not explicitly identified as such.

The next group of input records (numbers 6 through 87 in the example) contains information on the individual reactions in the mechanism, with the format of each record being identical. Each input record contains information for a single reaction. For each reaction, up to three reactants are allowed, each identified by an alphanumeric code no more than four characters in length. The code for each reactant is contained in one of three fields, field one corresponding to columns 1-4, field two to columns 7-10, and field three to columns 13-16. If only two reactants are associated with the reaction, the third field is left blank. Similarly, for a unimolecular reaction, fields 2 and 3 are left blank. The user supplied reaction identification number is contained in columns 17-18. (Since these are integer numbers, they must be right justified.) To allow for reaction numbers greater than 99, a modulus factor may be entered in column 24. If a non-zero entry is found in this column, the reaction number will be modified internally within the program and displayed upon output as a three digit number:

$$N_R = (MF \times 100) + N_{IN} \qquad (3\text{-}9)$$

where

N_R = user defined reaction number

MF = modulus factor (1 or 2), column 24

N_{IN} = input reaction number supplied in columns 17-18

The number of products of each chemical reaction are limited to four, and the product names are coded in four fields following the modulus number: columns 25-28, columns 33-36, columns 41-44, and columns 49-52. Again, the products are entered starting with the left-most field, leaving all fields not used blank. Columns 55-64 contain the rate constant for non-photolytic reactions, or the multiplicative constant for photolytic reactions. If an exponential format is used, then the entry must be right justified. All rate constants must be in ppmV-minute units (e.g., min^{-1} for unimolecular reactions, $ppmV^{-1}min^{-1}$ for bimolecular reactions, and $ppmV^{-2}min^{-1}$ for trimolecular reactions). Finally, the last field contains the activation energy, if available, in units of °K in columns 66-72.

In the example shown in Table 3-3, the chemical reactions are contained in input records 6 through 87 (i.e., a total number of 82 reactions). To illustrate the format discussed above, consider input record number 18. The user defined reaction number for this reaction is 13, and the reaction itself is

$$HO_2^{\cdot} + NO \dashrightarrow NO_2 + OH^{\cdot} \qquad (3\text{-}10)$$

where $HO_2^{\cdot}$ and $OH^{\cdot}$ have been represented by HO2 and OH. The rate constant for this reaction is 1.2×10^4 $ppm^{-1}min^{-1}$, and no activation energy is specified.

3.2.2 City-specific Inputs

Eight options are available to the user for supplying city-specific input information to OZIPM-2. These data permit the user to set the light intensity for photolytic reactions, and specify dilution, post-0800 emissions, transported pollutant concentrations, reactivity of the organic mix, and the initial NO_2/NO_x ratio. Many of these options are identical to those used in OZIPP, and these will only be briefly described here. The user may wish to refer to Reference 6, the OZIPP User's Manual, for more information on any specific option.

3.2.2.1 Light Intensity (PLACE)

The rates of all photolytic reactions vary in accordance with the diurnal change in sunlight intensity, and these are set by means of the PLACE option. (The OZIPM-2 inputs for this option are identical to those used in OZIPP). The first four characters of the code word PLACE must be located in columns 1-4. Numeric fields 1 through 6 on the PLACE input record contain, in this order, city latitude, city longitude, city time zone, year, month, and day. Units for latitude and longitude are degrees north and degrees west, respectively. The time zone is identified by one of the following numerical codes:

OZIPM-2 Input	Time Zone
5.0	Eastern Daylight Time
6.0	Central Daylight Time
7.0	Mountain Daylight Time
8.0	Pacific Daylight Time

(Conversion to standard time can be accomplished by adding 1 to the above numbers.) Numerical equivalents of year, month, and day would be used for the date. For example, the date June 21, 1984 would be represented as follows: year = 1984, month = 6, and day = 21.

The preset default values for this option correspond to the 1975 summer solstice (June 21) in Los Angeles, California (i.e., latitude = 34.058° north, and 118.250° west). Any one, or all, of these values may be overridden. If any non-zero entry is made for latitude or longitude, then one additional input record *must* be supplied. This second input record is of alphanumeric format (columns 1 through 24), and permits the user to supply the name of the city to the program for report generation.

3.2.2.2 Dilution (DILUTION and MIXING)

Dilution in OZIPM-2 occurs as a result of the mixing height rising from its early morning minimum to its afternoon maximum. Two separate options are available for providing the dilution related model inputs - DILUTION or MIXING. The DILUTION option is identical to that contained in OZIPP (Version 2), but the MIXING option is a new feature that permits the user to specify any particular diurnal pattern. Note that defaults have been preset for the DILUTION option, but use of the MIXING option requires that input be provided (i.e., there are no defaults for MIXING).

With the DILUTION option, the diurnal change in mixing height follows the characteristic curve developed by Schere and Demerjian[11] (see Figure 2-1). The inputs associated with this option include the initial (morning) mixing height, the final (maximum afternoon) mixing height, the time at which the mixing height begins to rise, and the time at which the mixing height ceases rising any further. These values are placed in the first four numeric fields on the input record with the DILUTION code word. Units for the mixing heights are unimportant, provided that the initial and final values are consistent and the number of significant figures is sufficient for adequate resolution. Starting and ending times should be in 24-hour format, Local Daylight Time for those areas on Daylight Savings Time (e.g., 0800 and 1500).

The preset default values for the DILUTION option correspond to Los Angeles-type conditions, with a very small growth in the mixing height over the day. Specifically, the initial morning mixing height is set at 510 meters, and the maximum afternoon mixing height at 630 meters. Under default operation, the mixing height growth begins with the start of the simulation (0800 LDT), and ends at the time corresponding to 70% of the daylight hours. The default timing can be used with city-specific inputs on mixing heights by simply overriding the mixing height values, and leaving the time inputs blank. Alternatively, the user may provide inputs on the times of the start and stop of mixing height rise. In the latter case, the timing will conform to the user inputs, and the shape of the characteristic curve will be modified to fit these specifications.

The MIXING option allows the user to specify any particular diurnal mixing height profile when such data are available. The inputs include the total number of hours of dilution, plus mixing heights at hourly intervals. In general, if n hours of dilution are specified, then n+1 mixing heights must be provided on input. Up to 15 hours of dilution may be specified, but the starting mixing height must always correspond to the simulation starting time. If a simulation calls for no dilution for several hours, then the same mixing height should be given for those hours. (Note that the mixing height cannot be zero, nor can it be lower than a value used for any previous hour.) As with the DILUTION option, the mixing heights may be specified in any particular units, but must be consistent for all hours.

The number of input records associated with the MIXING option depends on the total number of hours of dilution that are specified. The first input record contains the MIXING code word, followed by the total number of hours of dilution in the first numeric field. The mixing heights themselves are entered in the remaining fields in chronological order, i.e., the starting mixing height is entered in field 3, the mixing height at the end of the first hour in field 4, etc. If more than five hours of dilution are specified, then the mixing heights are continued on a second input record which must immediately follow the MIXING record.

3.2.2.3 Post-0800 Emissions (EMISSIONS and MASSEMISS)

The OZIPM-2 model is a simplified photochemical trajectory model built around a theoretical column of air that moves with the wind. During the course of the trajectory, fresh emissions of VOC and NO_x can be injected into the column. In OZIPM-2, as in OZIPP, the emissions data are expressed as a set of hourly emission fractions that are multiplied times the initial NMOC and NO_x concentrations, and adjusted for the changing height of the column. The resultant concentrations of these pollutants are added each hour to represent the effects of the emissions that occur subsequent to the simulation starting time. Unlike OZIPP, however, OZIPM-2 offers two options for specifying these data: the EMISSIONS option which is identical to that contained in OZIPP, and the MASSEMIS option which is a new feature.

EMISSIONS. With the emissions option, hourly emission fractions for NMOC and NO_x are supplied directly to the program. (Procedures for estimating these fractions have been discussed in References 3 and 8). A single set of emission fractions may be entered for both NMOC and NO_x, or a separate set may be supplied for each pollutant. Consider first, a case in which only one set of emission fractions is being used for both NMOC and NO_x. The EMISSIONS option is activated by placing the code word EMISSIONS in the first field (columns 1-10). The first numeric field of this record (columns 11-20) contains the total number of hours for which fractions are to be input, coded as a positive number. Numeric fields 2 through 6 (i.e., columns 21-30, 31-40, 41-50, etc.) contain the emission fractions for the first five hours. The first fraction is for the first hour of the simulation, the second is for the second hour of the simulation, and so forth. If more than five hours of emission fractions are being entered, then the remaining fractions are coded on an input record immediately following the EMISSIONS input record, with the sixth emission fraction placed in columns 1-10, the seventh in columns 11-20 and so on. The total number of hours permissible is limited to 15.

The procedure for coding two sets of emission fractions is analogous to the procedure just discussed. Instead of coding the total number of hours as a positive number, however, it is coded as a negative number. The NMOC fractions are then entered in exactly the same manner as described above. The NO_x emission fractions, however, are coded beginning with a new input record that immediately follows the input record with the last NMOC fraction. The fraction for the first hour is entered in columns 1-10, the second in columns 11-20 and so on. If more than seven hours of fractions are to be entered, the remaining fractions are entered in the next input record. Note that the total number of hours specified applies equally to both the NMOC and NO_x fractions, and the NMOC fractions must always precede the NO_x fractions.

If emission fractions are to be specified for only one pollutant (i.e., VOC or NO_x), then the emission fractions for the other pollutant could be entered as a set of zeros. OZIPM-2 has been set up, however, such that a negative entry for the first emission fraction of any set indicates that all fractions for that pollutant are zero, and no additional input records are required. Consider, for example, a case in which ten hours of emission fractions are desired, with all NMOC fractions assumed to be zero. The first input record would contain the code word EMISSIONS in columns 1-10, and would have a -10.0 coded in columns 11-20 (i.e., numeric field 1). Then, any negative number could be coded in the second numeric field to indicate that all of the NMOC emission fractions are to be zero. The next input record would contain the first seven NO_x emission fractions (not the VOC emission fractions for hours 6 through 10).

The last three NO_x emission fractions (hours 8 through 10) would be coded on the input record immediately following the one with the first seven. Alternatively, if only VOC emission fractions are to specified, with all NO_x fractions set to zero, the VOC fractions would be coded normally, but the first NO_x fraction would be set to a negative number.

MASSEMISS. Reference 8, Guidance For The Use Of City-specific EKMA In Preparing Ozone SIPs, contains one approach for computing post-0800 emission fractions. In this approach, an hourly emission fraction is computed as the ratio of a mass emission density to the emission density required to generate the concentration initially within the column (see equation 2-1). Since emission fractions are calculated routinely for several hours, a number of repetitive calculations are often required. The MASSEMISS option is intended to facilitate this process by performing the repetitive calculations internally. Inputs required by the MASSEMISS option include the initial mixing height (in meters), the initial NMOC concentration (ppmC), initial NO_x concentration (in ppm), and hourly emission densities for both VOC and NO_x. The first three inputs are used to calculate the emission density required to generate the initial concentrations that are specified (i.e., the denominator of equation 2-1). The hourly emission densities are determined from emissions inventory data and the space-time track of the trajectory (see for example Reference 8). Hourly emission fractions for each pollutant are then computed according to equation 2-1.

The format of the MASSEMISS inputs is similar to that of the EMISSIONS inputs. Again, the option is activated with the appropriate code word. The first numeric field must then contain the total number of hours of emissions. The second and third numeric fields must contain the initial NMOC and NO_x

concentrations to be used in the emission fraction calculations. Finally, the fourth field on this record contains the initial mixing height, in meters.

The hourly emission density inputs are coded on input records immediately following the MASSEMISS input record. The first of these input records contains the first seven VOC emission densities. If more than seven are being used, the entries are continued on a subsequent input record. The NO_x emission density inputs always begin on a new input record, and immediately follow the VOC inputs. Again, more than one record is required for more than seven hours of emissions.

3.2.2.4 Reactivity Factors (REACTIVITY)

The REACTIVITY option is used to supply information on the reactivity of NMOC and NO_x. The NO_x reactivity factor is simply the fraction of initial NO_x that is NO_2. It could be determined, for example, from 6-9 a.m. measurements of NO and NO_2 taken in the urban core.[8] If such a city-specific value is to be used, the appropriate entry should be placed in the second numeric field of the REACTIVITY input record (i.e., columns 21-30). Or, alternately, the default value of 0.25 may be selected instead.

NMOC reactivity data consist of a set of carbon fractions that are used to apportion total NMOC into the individual organic classes contained in the mechanism. The apportionment process is carried out for both the NMOC concentration initially present in the theoretical column (i.e., the initial NMOC concentration), and the NMOC concentrations that are added to reflect the effect of emissions injected into the column along the trajectory. Note that the same apportioning factors are used for both processes. The apportioning factors themselves may be obtained in several ways. First, a particular mechanism may have a set of recommended default factors that have been determined experimentally. Such is the case with the DODGE mechanism. For other mechanisms, the apportioning factors can be derived from detailed emission inventories in which VOC emissions have been tabulated by organic compound, or from analyses of captured air samples in which individual organic species concentrations are quantified. In some cases, recommended default values derived from surveys of such data may be available (e.g., recommended default apportioning factors are provided for the Carbon-Bond 3 mechanism in References 9 and 14).

Whichever approach is used to derive the apportioning factors, the procedure and results will likely be mechanism dependent. Nevertheless, some special considerations in deriving these inputs warrant further discussion. The apportioning scheme used in OZIPM-2 is applied to total concentrations of NMOC which are typically derived from ambient measurements of organic compounds. Because oxygenated organic compounds are often poorly detected in these measurements, the resultant ambient concentrations are considered to be more representative of nonmethane hydrocarbons (i.e., NMOC less oxygenated species such as aldehydes, ketones, etc.). As a consequence, many apportioning factors that have been derived for use with OZIPP or OZIPM-2 sum to a number slightly greater than 1.0 (e.g., 1.04 or 1.05) to account for the oxygenated compounds.[2,9,14] Furthermore, in several of the OZIPM-2 output reports, the terms "TOTAL HC" and "ALDEHYDE FRACTION" appear. In this context, "TOTAL HC" always refers to the sum of all organic groups that have been identified as "hydrocarbons." The "ALDEHYDE FRACTION" is determined by the total aldehyde concentration expressed relative to "TOTAL HC."

In the DODGE mechanism, organic compounds are represented by four separate species. "Hydrocabons" are represented by propylene and butane, and the "aldehydes" by formaldehyde and acetaldehyde. As noted above, recommended apportioning factors have been developed, and are preset as default values in OZIPM-2. Specifically, these values are: 25% of the OZIPM-2 hydrocarbon is propylene, 75% is butane, and 5% of the OZIPM-2 hydrocarbon is added as total aldehydes (OZIPM-2 splits the aldehydes into formaldehyde and acetaldehyde in a 60%/40% basis).

The organic REACTIVITY inputs are activated with two fields on the REACTIVITY input record. In the first numeric field (i.e., columns 11-20), the number of OZIPM-2 "hydrocarbon" species is coded. (This would normally be the same number as that used for the number of hydrocarbon species entered for the MECHANISM option.) Similarly, the number OZIPM-2 "aldehyde" species is coded in the third numeric field (columns 31-40). The apportioning factors for the OZIPM-2 "hydrocarbon" species are placed in the first input record immediately following the REACTIVITY input record. These apportioning factors (or carbon fractions) must be expressed on a carbon basis (not a molecular basis), and must be entered in the same order as used in the MECHANISM option inputs. The fractions themselves are coded in seven numeric fields, each ten columns wide, beginning with column 1. If more than seven "hydrocarbon" species are used in the mechanism, then the inputs are continued on the next input record. The aldehyde carbon fractions are placed on a new input record immediately following all input data for the "hydrocarbon" fraction. If aldehydes are not included in the mechanism, then the "aldehyde" input record must be omitted.

3.2.2.5 Transported Pollutants (TRANSPORT)

In OZIPM-2, as in OZIPP, pollutant transport into a city from upwind areas can be considered. Such transport can occur in two different ways. First, pollutants may be transported in the surface layer, such that they are present within the theoretical column at the beginning of the model simulation.

Second, pollutants may be transported within air masses trapped above the mixed layer at night, and later entrained into the mixed layer as the mixing height begins to rise. In either case, the pollutants that can be considered include organics, NO_x and ozone. Information on methods for estimating the levels that are transported is included in References such as 8 and 9.

Default assumptions in OZIPM-2 correspond to no transport of any pollutant. The method for overriding the defaults depends to some extent on the pollutants under consideration and the chemical mechanism that is being used. When ozone transport is to be accounted for explicitly, the first and second numeric fields of the TRANSPORT option input record are used to enter the concentrations of ozone (in ppm) transported in the surface layer and in the layer aloft, respectively. Similarily, numeric fields five and six are used for surface and aloft transport of NO_x, respectively (also in ppm). (Note that all transported NO_x is assumed to be NO_2.) The remaining two fields (numeric fields 3 and 4) are used for information on the transport of organic compounds. With the DODGE mechanism, the total concentrations (in ppmC) of NMOC transported in the surface layer and aloft are entered in these two fields, with surface layer transport in field 3 (columns 31-40) and aloft transport in field 4 (columns 41-50). Any combination of pollutant transport (i.e., surface versus aloft) and pollutant (i.e., O_3, NMOC or NO_x) is permissible.

When a mechanism other than DODGE is being used, the format for the NMOC inputs is somewhat different. Instead of entering NMOC concentrations in numeric fields 3 and 4, the number of "hydrocarbon" species, coded as negative number, is used as a flag. A negative entry in numeric field 3 signifies surface transport, and a negative entry in field 4 signifies transport aloft. In either case, the required NMOC input data are provided on subsequent input records. For surface layer transport, the total NMOC concentration aloft, in ppmC, is coded in the first numeric field of a new input record (i.e., columns 1-10). The remaining six fields on this record are used to supply the "hydrocarbon" carbon fractions that are needed to split transported NMOC into the individual organic groups of the mechanism. Again, the carbon fractions must be entered in the same order as in the MECHANISM option. Also, if more than six "hydrocarbon" species are being used, then the remaining carbon fractions are continued on the next input record. The carbon fractions for "aldehydes" are entered on a new input record, beginning in its first numeric field. If "aldehydes" are not in the mechanism, then this input record is omitted.

The input format for NMOC transported aloft is exactly the same as that for surface level transport (i.e., total NMOC concentration, followed by "hydrocarbon" carbon fractions, followed by "aldehyde" carbon fractions). If NMOC transport aloft is to be included (i.e., a negative number coded in numeric field 4 of the TRANSPORT input record), then the inputs for transport aloft must immediately follow all of the records containing the NMOC inputs for surface transport if they are present. Otherwise, they come directly after the TRANSPORT input record itself.

As indicated in the discussions above, the carbon fractions used for surface transport and transport aloft need not be the same, nor do they need need to be the same as the carbon fractions used with the REACTIVITY option. Thus, the composition of aged air masses associated with transport from upwind areas may be assumed to be different from the composition of the organics associated with fresh emissions. Also, use of the TRANSPORT option differs slightly from others with respect to its order in the input records. Since the number of "aldehyde" species must be defined before the TRANSPORT option is encountered when NMOC transport is being included and an alternate mechanism is being used, the MECHANISM option inputs must always precede the TRANSPORT option when both options are used.

3.2.3 Options for Program Control

The two categories of OZIPM-2 options that have previously been discussed allow the user to supply the program with information on the chemical mechanism and with city-specific information for some of the physical processes simulated by the model. Attention is now focused on those inputs associated with the options that cause the program to perform one of three major functions: (1) perform a single simulation, (2) generate an isopleth diagram, or (3) perform a VOC control calculation.

3.2.3.1 Single Simulation Option (CALCULATE)

The CALCULATE option directs the OZIPM-2 program to perform a single simulation. This option might be used, for example, to predict a single occurrence of peak ozone, or to gain more information about a simulation conducted under one of the other two modes of operation. In the CALCULATE mode, the user must supply the initial NMOC and NO_x concentrations that are used in the simulation. Under the default mode of operation, instantaneous pollutant concentrations (i.e., the concentration of any pollutant at a specific point in time) of major species are tabulated, and the maximum one-hour average ozone concentration occurring during the simulation is reported. Conceptually, these predicted concentrations represent the change in pollutant concentrations in the air mass that moves according to the user defined trajectory.* The user also has the option of displaying the instantaneous concentrations of all species in the mechanism, and computing the maximum one-hour average concentration of any pre-selected species.

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*The trajectory is ultimately determined by the starting location of simulation (which is used to establish the initial pollutant concentrations) and the path that the air parcel follows (which is determined by the user input post-0800 emissions).

The CALCULATE option is activated by means of an input record containing the code word CALCULATE in the first field (i.e., columns 1-10). The first numeric field (columns 11-20) contains the initial NMOC concentration, in ppmC, and the second field contains the initial NO_x concentration, in ppm. Under default operation, simulation output consists of a report showing the concentrations of hydrocarbons, aldehydes, NO_x, and ozone. These concentrations are reported at hourly intervals beginning with the simulation starting time. The maximum one-hour average concentration of ozone is also reported unless changed with the SPECIES option (discussed in Section 3.2.4.4). Finally, a line-printer plot showing the time-concentration profile of ozone (or the species selected with the SPECIES option) is produced.

Alternatively, the user has the option of requesting more information on the simulation results. Any non-zero entry coded in the third numeric field of the CALCULATE input record triggers the generation of a detailed output report. Included are the following:

- the rate constants used in the kinetic mechanism
- the photolysis rates for all photolytic reactions (as a function of time)
- concentrations of each species in the mechanism (as a function of time)
- the net rate of change of each species (as a function of time)
- the reaction rates of each reaction in the mechanism (as a function of time)

Unless changed by the user, the detailed information is reported for the time at which the simulation begins, and for 60 minute intervals thereafter. The user may control the report generation, however, by specifying the simulation time at which the reports are to begin, and the time increments for subsequent reports. (The information at the start of the simulation is always reported.) The initial report is controlled by entering the number of minutes after the simulation start at which the reports are to begin in the fourth numeric field (i.e., columns 41-50) of the CALCULATE input record. The time interval, in minutes, for subsequent reports is placed in numeric field (51-60) of the same input record. Since default conditions cause reports to be generated at hourly intervals, default values for both of these control variables are 60 minutes. As with the default mode, a line-printer plot showing the time-concentration profile of ozone, unless changed using the SPECIES option, is shown upon completion of all tabular reports.

3.2.3.2 Isopleth Diagram Option (ISOPLETH)

The generation of an isopleth diagram (see Figure 2-2 for an example) is activated by means of the ISOPLETH option. Under this mode, repeated simulations are conducted with differing initial concentrations of NMOC and NO_x, and the maximum one-hour average concentrations of a specified pollutant (default equals ozone) are determined. These discrete multiple simulations are in turn used to interpolate and plot the maximum one-hour average level of the species of interest as continuous functions of initial NMOC and NO_x concentrations. Since the post-0800 emissions are expressed relative to the initial concentrations, the diagram depicts graphically how the pollutant changes relative to changes in post-0800 emissions of NMOC and NO_x, as well as initial NMOC and NO_x concentrations.

In addition to the code word in the first field, the ISOPLETH option contains four numeric fields. The first two fields are used to control the scale of the abscissa (i.e., NMOC) and the scale of the ordinate (i.e., NO_x). The maximum NMOC concentration (in ppmC) to be used in the diagram is entered in the first field (i.e., columns 11-20), and the maximum NO_x concentration (in ppm) is entered in the second numeric field. (The origin of the diagram always corresponds to the point 0,0.) While any number may be used for the maximum NMOC or NO_x concentration, some consideration should be given to the scale divisions shown on the diagram. The scales of the abscissa and ordinate are divided into ten and seven divisions, respectively. Thus, only particular values of the maximum concentrations will produce divisions whose labels are even numbers. For example, to produce an easy to read diagram, the maximum NO_x concentration should be evenly divisible by seven (e.g., 0.07 ppm, 0.14 ppm, 0.21 ppm, etc.). Similar considerations should be taken into account when selecting the NMOC maximum concentration, which will be divided by ten to produce the diagram divisions.

In addition to fixing the scales of the diagram, the user may also control the specific isopleths that are plotted. As noted above, an ozone isopleth diagram is generated under default conditions. The program contains a set of default ozone isopleth values corresponding to 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36, and 0.40 ppm. The user may override these defaults by requesting up to 20 specific isopleths. First, the total number of isopleths desired is entered in the third numeric field of the ISOPLETH input record (i.e., columns 31-40). Second, the concentration levels of the desired isopleths are entered in the input record(s) that immediately follow the ISOPLETH option. Each record contains seven values corresponding to seven numeric fields which are ten columns wide. Thus, a request for one to seven isopleths would require one additional input record, a request for 8 to 14 would require two input records, and a request for 15 to 20 would require three additional input records.

When generating an isopleth diagram, some consideration should be given to insuring that the desired isopleths are evenly spaced on the diagram. For example, the particular scales chosen for the diagram and the city-specific inputs selected for the simulations may result in a situation in which a desired isopleth cannot be plotted on the diagram. Although the problem could be overcome by selecting different diagram scales in a trial and error mode, computer time can be saved by performing several CALCULATE simulations with candidate diagram NMOC and NO_x maxima. The resultant one-hour average concentrations produced by the CALCULATE simulations provide the user with an upper limit of the isopleths that can be plotted on the diagram. For example, suppose that it is desired to generate an ozone isopleth diagram containing two isopleths corresponding to 0.24 ppm and 0.12 ppm. Suppose a series of CALCULATE simulations were performed with candidate maximum NMOC and NO_x concentrations to be used for the diagram, and the following results obtained:

Simulation Number	Initial NMOC, ppm	Initial NO_x, ppm	Maximum one-hour Average ozone, ppm
1	0.5 ppmC	0.07 ppmC	0.16
2	1.0 ppmC	0.14 ppmC	0.30
3	2.0 ppmC	0.28 ppmC	0.40

Since the maximum ozone concentration corresponding to simulation 2 is greater than 0.24 ppm, these results suggest that the NMOC and NO_x values used in simulation 2 may be appropriate scaling parameters. Although the third simulation indicates that the selection of 2.0 ppmC and 0.28 ppm would also provide the desired isopleths, the higher predicted ozone concentration (0.40 ppm compared to the desired 0.24 ppm) suggests that the desired isopleths would be located well to the left on the diagram, thereby producing uneven isopleth spacing. Since a small number of CALCULATE simulations require less computer time than an ISOPLETH run, a considerable amount of computer time could be saved following this approach.

When selecting candidate scales for an ozone isopleth diagram, the user may wish to keep in mind the ultimate use for that diagram. Typically, it will be used in a VOC control calculation in which a design $NMOC/NO_x$ ratio is plotted on the diagram, and its intersection with a design ozone isopleth is located. The optimal diagram arrangement is one in which the design $NMOC/NO_x$ ratio is near the diagonal of the diagram, and the isopleth corresponding to the design ozone concentration is in the upper right quadrant of the diagram. Not only does this arrangement facilitate the use of the diagram, it also provides optimal utilization of the OZIPM-2 algorithm that is used in the diagram construction.

One additional ISOPLETH option is available to the OZIPM-2 user. As noted earlier, an isopleth diagram is produced by performing repeated simulations that generate the maximum, one-hour average concentrations that are used in the construction of the diagram. These simulation results are always summarized in tabular form showing the initial NMOC and NO_x concentrations used in the simulations, the ratio of these concentrations (i.e., $NMOC/NO_x$), and the maximum one-hour average that results. Any non-zero entry in the fourth numeric field of the ISOPLETH option causes the program to print the time of the center of the resultant maximum one-hour average as well (in minutes after the simulation start). In this mode, as well as in the default mode, the phrase "not max" will be printed whenever a maximum concentration is not reached. In the event a user desires to examine in more detail the conditions leading to a "not max" situation, a CALCULATE option may be run with the printed NMOC and NO_x concentrations leading to that situation.

Activation of the ISOPLETH option automatically generates a line-printer plot of the isopleth diagram. The user also has the option of generating an off-line plot (e. g., by CALCOMP) by means of the PLOT option. (The details of the PLOT option are discussed in Section 3.2.4.2.) When such a plot is desired, the PLOT option must precede the ISOPLETH option, and only one isopleth diagram can be generated per model run.

3.2.3.3 Control Calculation (EKMA)

A new feature of the OZIPM-2 program is its ability to perform a VOC emission reduction calculation without generating an ozone isopelth diagram. In this mode, the user must supply information on the base-case peak ozone level to be reduced (referred to here as the base ozone value), the $NMOC/NO_x$ ratio to be used in the calculation, and the percentage change in NO_x emissions. The calculations are performed in accordance with the procedures used to calculate control estimates from an ozone isopleth diagram. (The reader is referred to References 3, 8 and 9 for background.) Through an iterative search procedure, a base-case point is first located by finding the initial NMOC and NO_x concentrations (in the specified ratio) that produce the desired ozone concentration (within 0.0005 ppm). A post-control point is then found by first adjusting the base-case NO_x point to reflect the change in NO_x emissions input by the user, and then finding the initial NMOC concentration that, along with the adjusted NO_x concentration, will produce an ozone value of 0.12 ppm (again, within 0.0005 ppm). The VOC reduction estimate is then calculated as the percent change in NMOC concentration from the base-case point to the post-control point. (A more detailed discussion is included in Section 2.2.3).

The EKMA option is activated by an input record with the code word EKMA located in columns 1-4. The base ozone value is then placed in the first numeric field of the EKMA input record. The second numeric field of this record contains the NMOC/NO_x ratio. Note that defaults have not been included in the program, so these values must be entered by the user. The percentage change in NO_x emissions that is expected between the base-case and the post-control time periods is coded in the third numeric field. This value should be entered as the percent change. Thus, a positive entry corresponds to an increase, and a negative entry to a decrease. (For example, a 5% increase would be coded as 5.0, and a 5% decrease as -5.0.) The fourth numeric field is used to signify a change in transport conditions. If the same transport conditions are assumed for the base-case and post-control case, then this entry may be left blank. Otherwise, a numeric entry (e.g., 1.0) denotes that different transport conditions are to be used for the post-control case than for the base-case case, and these new values are coded in the next input record. The first two fields of this input record contain the surface and aloft ozone concentrations (in ppm), respectively. Similarly, the next two contain the surface and aloft NMOC transport levels (in ppmC), and the last two contain the NO_x surface and aloft transport levels (in ppm). The user should note that the structure of this input record is similar to that of the TRANSPORT input record, but if any entry is left blank, then the base-case transport level will be used for the post-control case. Also, no provisions are included for making any changes to the composition of NMOC used in the simulations (i.e., the same NMOC transport composition will be used for both base-case and post-control point).

As described above, the EKMA option causes the program to compute the VOC reduction (in percent) needed to lower the base ozone to 0.12 ppm. One additional option is available to the user to generate supplemental information.

An entry of 1.0 in the fifth numeric field of the EKMA option record causes the generation of a tabular report showing the change in ozone as a function of percentage change in VOC. Predicted ozone corresponding to VOC reductions of 10%, 20%, 30%, ..., and 100%, respectively, are printed. If a value of 2.0 is coded instead, the predicted ozone concentrations will also be written to a user defined file, which might be used for subsequent analysis or graphical display. One output record is written to the file for each EKMA option that is activated. The output format consists of 11 fields, each five columns wide. The first field (columns 1-5) contains the base-case ozone value. The remaining ten fields contain the ozone predictions corresponding to the VOC reductions of 10%, 20%, 30%, ...100%, in that order.

3.2.4 Miscellaneous Options

The major options governing OZIPM-2 operation have been discussed in the previous sections. Additional options that are available to the user to control the model simulations and program operation are described below.

3.2.4.1 Title (TITLE)

A default title, "Standard Ozone Isopleth Conditions," is printed on all output reports unless overridden by the user with the TITLE option. To activate this option, the code word TITLE is coded in the first field of this option input record. The title to be used on all subsequent output reports is coded on an input record immediately following the TITLE input record. Any entry made in columns 1-72 of this record will be included as part of the title.

3.2.4.2 Offline Plot (PLOT)

An offline plot of an isopleth diagram may be generated whenever the ISOPLETH option is invoked. Any plotting package that uses the standard CALCOMP software may be used, but file handling and subroutine linkage must be carried out by the user. Additional information on the latter is contained in Section 4.3.2.

When generating an offline plot, the user has a number of options available. First, the physical size of the diagram may be controlled with the third and fourth numeric fields of the PLOT option input record. Under default operation, the diagram that is generated will be 8.5 inches wide by 5.95 inches high. A different sized diagram may be generated by entering the length of the abscissa (in inches) in the third numeric field, and the length of ordinate (in inches) in the fourth numeric field. The size of the title characters, axes labels, isopleth labels, and axes tickmarks are controlled by numeric fields five and six. The default size for all title characters and axes labels is 0.10 inches, but can be overriden by an entry (in inches) in the fifth numeric field. Similarly, the size of the ozone isopleth labels and tick marks (default = 0.07 inches) is controlled by the sixth numeric field. The first numeric field controls the location of the label for each isopleth that is plotted. Permissible values range from 0.1 to 0.8, and refer to the relative arc length along an isopleth at whch the isopleth label is positioned. The default for this parameter is 0.6. Except for the positioning factor controlling the location of isopleth labels, proportional changes to all parameters is recommended when resetting any of the defaults.

The only other PLOT option available to the user is one that activates a grid overlay on the diagram, but it is specific to the plotting package being used. For CALCOMP plotters, any positive entry in the second numeric field generates a grid overlay. The grid overlay will be of a different color if the user has access to this CALCOMP option. For users having access to a matrix plotter (e.g., VERSATEC), the thickness and pattern (e.g., dot-dash) of the grid is controlled by entering a negative number (non-zero) in the second numeric field. The pattern and texture of the grid network is controlled by the absolute value of the entry, which varies with different plotting systems.

3.2.4.3 Simulation Length (TIME)

The default simulation length for all simulations is ten hours, starting at 0800 LDT and ending at 1800 LDT. The default simulation length can be modified by invoking the TIME option. The first numeric field on this input record is for the starting time, and the second numeric field is for the ending time. In both cases, 24-hour clock time should be entered (e.g., 0700, 2000, etc.). Note that when the starting time is changed, the city-specific inputs for EMISSIONS and MIXING are expressed relative to the new starting time. For example, if the starting time is changed to 0700 LDT, then the first hour of emissions refer to the period 0700 to 0800 LDT. Also, the total length of the simulation is limited to 15 hours.

3.2.4.4 Isopleth Diagrams For Alternate Species (SPECIES)

Under default operational mode, an ozone isopleth diagram will be generated when the ISOPLETH option is invoked, and the maximum one-hour average ozone concentration will be computed with the CALCULATE option. To generate an isopleth diagram for another species, the user may activate the SPECIES option by entering the code word in an input record, and positioning this input record before the ISOPLETH option. The species that is desired is entered on an input record that immediately follows the SPECIES input record. The species code word that is used in the chemical mechanism must be entered in columns 1-4 of this input record, and must be left justified. Unless the concentration values of the species correspond to typical ozone levels, the user may also wish to modify the ISOPLETH option inputs in order to produce isopleths that correspond to typical levels of the species of interest. Finally, inclusion of the SPECIES inputs before a CALCULATE option causes OZIPM-2 to report the maximum, one-hour average concentration of the species of interest instead of ozone, and to produce a line-printer plot showing the corresponding time-concentration profile.

3.2.4.5 Setting Initial Concentrations (INITIAL)

Initial concentrations of all species other than NMOC, NO_x and ozone are assumed to be zero at the start of the simulation unless overridden by the INITIAL option.* The INITIAL option is activated by coding INITIAL in the first field of the INITIAL input record, and by entering in the first numeric field the total number of species whose initial concentrations are to be reset. Up to 80 species' concentrations can be specified at one time. The mechanism code names of the species whose concentration are to be initialized are entered on an input record immediately following the INITIAL input record. The first species name is entered in the first four columns of the first numeric field (columns 1-4), the second in the first four columns of the second numeric field (i.e., columns 11-14), and so forth. Up to seven species names can be coded on any one input record, and all species names must be left-justified in their respective fields. The initial concentrations of the designated species are entered in a set of input records that immediately follow the records containing the species names. Entries must be in the units of molar concentration (i.e., ppmV), and must be in the same order as named in the first set of inputs. The concentration of the first species is coded in the first numeric field of a new input record, the second in the second numeric field, etc. Again, seven concentrations can be coded on any one input record, with the remaining concentrations coded on as many additional input records as needed.

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*Initial concentrations of organic compounds, NO, NO_2 and ozone cannot be controlled by this option.

3.2.4.6 Controlling Simulation Accuracy (ACCURACY)

A number of options are available to the user that affect the accuracy used in single simulations and in the construction of isopleth diagrams. These options are identical to those available in OZIPP, and will only be briefly summarized here. The reader may wish to refer to the OZIPP User's Manual for additional information. Although the default values preset in OZIPM-2 will be adequate for most applications, the discussion below is included for completeness.

The ACCURACY option permits the user to control the numerical accuracy in generating isopleth diagrams by using more or fewer simulations, more or less accuracy in interpolation, etc. As described in Section 2.2.2, a series of simulations are performed at several points located along radials emanating from the origin when an isopelth diagram is generated. The number of radials, and the number of points along those radials, can be controlled by the user. First, consider the radials. Under default operation, 11 radials are used in diagram generation. The user may alter this value by entering any odd number, from 1 to 19, in the first numeric field of the ACCURACY input record. Similarly, the number of points selected along those radials is controlled with the second numeric field. The default value of 5 points per radial can be overridden by placing any number between 1 and 8 in this field. It should be added that these parameters affect the computer time required to generate an isopleth diagram, so some adjustments to that parameter may be required if the number of points is increased significantly (see also Section 4.3.2).

Numeric fields 3, 4 and 5 are used for parameters that affect the accuracy of the numerical integration, and the interpolation and plotting that is carried out in generating a diagram. The error tolerance for the numerical integration is located in the third numeric field. The default value is 0.01, with smaller values increasing accuracy and larger values reducing accuracy. Permissible values range from 0.1 to 0.00001. Hyperbolic spline tension factors are controlled in numeric fields 4 and 5, with the fourth field used for interpolation tension, and the fifth field for plotting tension. The default values for both are 1.0. Higher numbers lead to straight lines, and lower numbers to cubic splines. Acceptable values range from 0.001 to 50.

The last numeric field in the ACCURACY input record can be used to conserve computer time by halting all simulations when the one-hour average concentration of ozone (or the species selected with the SPECIES option) reaches its maximum value. It should be noted that the use of this option runs the risk of missing "double ozone peaks" (i.e., conditions in which predicted ozone peaks, falls off, and then peaks again in a single simulation), and is not generally recommended. Nevertheless, it can be invoked by placing any non-zero entry in the sixth numeric field of the ACCURACY input record.

3.2.4.7 Using Previous Simulation Results (ALREADY)

The ALREADY option is included to allow the user to make use of previous simulation results, and thus potentially save computer time. This option might be used, for example, to restart a run that terminated due to a time restriction, to produce an off-line plot of an isopleth diagram generated under a prior run, or to alter the tension factors used in a prior run. Whenever this option is invoked, all other model inputs used in the previous run and the desired run must be identical. The savings in computer time result from the program not having to duplicate single simulations performed in the prior run, since these are provided as model inputs.

The first numeric field of the ALREADY input record contains the total number of isopleth diagram simulations that were completed in the prior run. The simulation results themselves are entered on a set of input records that immediately follow the ALREADY option, and may be obtained from the tabular report produced in the previous run. One simulation result is entered per record in the order that they were performed in the first run. The required entries include the initial NMOC concentration (numeric field 1), the initial NO_x concentration (numeric field 2) and the resultant maximum, one-hour average ozone concentration (or the concentration of the species of interest if the SPECIES option is used) in numeric field 3. Note that the total number of such input records must equal the number specified on the first numeric field of the ALREADY input option.

3.3 MULTIPLE ISOPLETHS OR CALCULATES

As mentioned earlier, the order of the OZIPM-2 option input records is not usually critical, so long as the appropriate inputs precede a functional option such as ISOPLETH or CALCULATE. Nevertheless, errors will be kept to a minimum if the ordering scheme shown in Figure 3-1 is used. Again, all input records associated with any particular option must be grouped together, and options that are not used may be omitted. A blank input record stops program operation.

The structure of OZIPM-2 also permits multiple operations to be performed in a single model run. One isopleth diagram is produced for each ISOPLETH option included with the inputs. Likewise, a single simulation is carried for each occurrence of a CALCULATE option, and a single VOC control calculation is performed for each EKMA option. Thus, for example, all three operations could be

Mechanism Inputs	MECH	FIRST
Simulation Options	TITLE PLOT TIME SPECIES INITIAL ACCURACY ALREADY	
City-specific Inputs	PLACE DILUTION OR MIXING REACTIVITY EMISSIONS OR MASSEMISS TRANSPORT	
Program Operation	CALCULATE ISOPLETH EKMA	LAST
Program Halt	blank record	

Figure 3-1. Example Order For OZIPM-2 Inputs.

performed in one run by including CALCULATE, EKMA and ISOPLETH input records at the end of the set of input record options. Further, the same operation can be performed in a single model run, but using different city-specific (or other inputs). The major consideration here is that an OZIPM-2 option, once activated, remains in effect until respecified.* As an example, consider the recommendation contained in Reference 8 for computing VOC reductions for the five days with the highest ozone levels at any particular site. Assume, further, that a mechanism other than DODGE is to be used. All the required operations could be performed in one model run using the input structure shown in Figure 3-2. Note that the MECHANISM option is activated just once, and thus remains in effect for all subsequent model simulations. The first EKMA option causes a VOC control calculation to be performed using the city-specific inputs for Day 1, but these values are then replaced with those for Day 2 when the second EKMA option is encountered.

Setting up multiple operations in a single run, however, requires consideration of some additional factors. First, the required computer time will be roughly proportional to the time needed for one option. Thus, for example, performing five EKMA calculations will take roughly five times as long as performing one EKMA calculation. Second, the PLOT option, once activated, cannot be turned off. In fact, if multiple off-line isopleth diagrams are desired, then these runs should be made separately, although any number of EKMA calculations and CALCULATE simulations may be included in the same run with the ISOPLETH and PLOT options. Finally, if the ALREADY option has been used to restart an ISOPLETH operation, it must be deactivated before starting the next

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*Note that if the default value for a particular variable is desired in place of a value specified earlier, then the default value must be respecified by coding its value on the appropriate input record.

MECH
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city-specific inputs for Day 1
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EKMA
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city-specific inputs for Day 2
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EKMA
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city-specific inputs for Day 3
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EKMA
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city-specific inputs for Day 4
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EKMA
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.
.
city-specific inputs for Day 5
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.
.
EKMA
blank record

Figure 3-2. Schematic Diagram Indicating Multiple Runs.

ISOPLETH operation. This may be done by including another ALREADY input record, after the first ISOPLETH option record, with a zero (or blanks) entered in its first numeric field.

4.0 USER'S GUIDE

This chapter describes the specific formats that are used for entering the model inputs discussed in the previous chapter. Also included are explanations of error messages and warnings that may be generated by the program, discussions related to the computer requirements associated with running the model, and example job control language.

4.1 FORMATS FOR INPUT DATA

Tables 4-1A through 4-1R contain the input formats for each of the 18 OZIPM-2 options. The order corresponds to that recommended in Section 3.3 (see Figure 3-1). Each option is always activated by placing its four letter code (e.g., MECH, PLAC, etc.) in columns 1-4 of the input record. Each input record has up to six numeric fields that begin in column 11, and are 10 columns wide. Unless otherwise noted, numerical entries made in these fields should always be coded with a decimal point, even if they are integral values. They may, however, be placed anywhere in the field. In the event that a field is too small to contain an entry, E-format (e.g., 1.0E02 for 100) may be used, but the entry must be right-justified within the field.

Some options require additional input records that must immediately follow the input record with the option code. With a few exceptions (e.g., the MECHANISM option), these records contain seven, 10-column, numeric fields that begin in column 1. The same coding convention is used for these fields, i.e., all entries should be coded with a decimal point, they may be located anywhere within the field, and any entry made with E-format must be right-justified within the field. In a few instances, integer values are required, and these must also be right-justified. Alphanumeric data required by the MECHANISM, SPECIES and INITIAL must be left-justified, however.

TABLE 4-1A
INPUT FORMAT FOR MECHANISM OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
MECHANISM			Used to provide inputs for an alternate kinetic mechanism. This option is not required when the default DODGE mechanism is to be used.
	1	1- 4	MECH
		11-20	The identification number of the last reaction (max=200.)
		21-30	The number of photolytic reactions in the mechanism (max=8.)
		31-40	Number of "hydrocarbon" species in the mechanism (max=10.)
		41-50	Number of "aldehyde" species in the mechanism (max=4.)
		51-60	Temperature (in degrees k) at which rate constants are determined (DF=303.)
		61-70	Number of photolytic reactions whose rates are expressed relative to NO_2 photolysis (max=8.)
	2*	1-10	Identification number of first photolytic reaction
		11-21	Identification number of second photolytic reaction

*If additional entries are required, they are continued on an input record immediately following the one with the first set of entries, using the same format.

TABLE 4-1A (continued)
INPUT FORMAT FOR MECHANISM OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
MECHANISM (cont'd)			
		⋮	
		71-80	Identification number of seventh photolytic reaction
	3*	1-10	Identification number of first photolytic reaction whose rate is proportional to NO_2 photolysis
		11-20	Identification number of second photolytic reaction whose rate is proportional to NO_2 photolysis
		⋮	
		61-70	Identification number of seventh photolytic reaction whose rate is proportional to NO_2 photolysis
	4*	1-4	Alphanumeric code for first "hydrocarbon" species, left-justified
		11-14	Alphanumeric code for second "hydrocarbon" species, left-justified
		⋮	

*If additional entries are required, they are continued on an input record immediately following the one with the first set of entries, using the same format.

TABLE 4-1A (continued)
INPUT FORMAT FOR MECHANISM OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
MECHANISM (cont'd)			
		61-64	Alphanumeric code for seventh "hydrocarbon" species, left-justified
	5*	1-10	The carbon number for the first "hydrocarbon" species
		11-20	The carbon number for the second "hydrocarbon" species
		. . .	
		61-70	The carbon number for the seventh "hydrocarbon" species
	6** (optional)	1-4	Alphanumeric code for the first "aldehyde" species
		11-14	Alphanumeric code for the second "aldehyde" species
		. . .	
		31-34	Alphanumeric code for the fourth "aldehyde" species

---

[*] If additional entries are required, they are continued on an input record immediately following the one with the first set of entries, using the same format.

[**] Optional records 6 and 7 are included only if the mechanism contains "aldehyde" species explicitly identified as such.

TABLE 4-1A (continued)
INPUT FORMAT FOR MECHANISM OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
MECHANISM (Cont'd)			
	7* (optional)	1-10	Carbon number for first "aldehyde" species
		11-20	Carbon number for second "aldehyde" species
		. . .	
		31-40	Carbon number for fourth "aldehyde" species
	8**	1-4	Alphanumeric code for first reactant, left-justified
		7-11	Alphanumeric code for second reactant, left-justified
		13-16	Alphanumeric code for third reactant, left-justified
		17-18	Identification number of reaction, any number between 0 and 99 (but 0 allowed only if next number is non-zero); right-justified integer

---

*Optional records 6 and 7 are included only if the mechanism contains "aldehyde" species explicitly identified as such.

**The kinetic mechanism inputs begin with this record. One record is included for each reaction, with all records having the same format.

TABLE 4-1A (continued)
INPUT FORMAT FOR MECHANISM OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
MECHANISM (Cont'd)			
		24*	Modulus factor for reaction identification number; permissible values are 0 (or blank) 1 or 2 (2 is only allowed when the reaction identification number is zero)
		55-64	The rate constant at 298°K, or the multiplicative constant for photolytic reactions; right-justified if E-format is used
		66-72	Activation energy, in °K, right-justified if E-format is used

*The modulus factor is used to redefine the reaction identification number if an entry is made that is greater than zero. For example, a reaction with identification number 48 (columns 17-18) would be identified as reaction number 148 if the modulus factor were 1.

TABLE 4-1B
INPUT FORMAT FOR TITLE OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
TITLE			Used to supply a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions."
	1	1- 4	TITL
	2	1-72	The title can be placed anywhere in columns 1-72

TABLE 4-1C
INPUT FORMAT FOR PLOT OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
PLOT			Activates the drawing of the isopleth diagram on an offline plotter
	1	1- 4	PLOT
		11-20	Scaling factor for the location of labels for each isopleth. The value should be between 0.1 and 0.8; DF=0.6.
		21-30	If non-zero, a grid is overlaid on the diagram. If the value is positive and non-zero, a grid is overlaid on the diagram using a different color pen (if available). If the value is negative, a grid with lines of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and texture.
		31-40	Length (in inches) of the abscissa (NMOC scale) of the isopleth diagram; DF=8.5
		41-50	Length (in inches) of the ordinate (NO_x scale) of the isopleth diagram; DF=5.95.
		51-60	Sizes (in inches) of the numbers to be printed on the axes and of the characters in the title; DF=0.10.
		61-70	The sizes (in inches) of the labels on isopleths and the division marks on the axis; DF=0.07.

TABLE 4-1D
INPUT FORMAT FOR TIME OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
TIME	Used to reset starting and ending times for model simulations		
	1	1- 4	TIME
		11-20	Starting time for simulations, 2400 hour format (DF=800.)
		21-30	Ending time for simulations, 2400 hour format (DF=1800.) (Note: maximum difference between start and end time is 15 hours).

TABLE 4-1E
INPUT FORMAT FOR SPECIES OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
SPECIES		Used to plot isopleths for any species in the mechanism, or determine maximum one-hour average concentration and plot time-concentration profile of species with CALCULATE option (DF=03)	
	1	1- 4	SPEC
	2	1- 4	Alphanumeric code of species of interest, left-justified

TABLE 4-1F
INPUT FORMAT FOR INITIAL OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
INITIAL			Used to specify initial concentrations of species other than organics, NO, NO_2, or ozone
	1	1- 4	INIT
		11-20	Number of species whose initial concentrations are to be reset (max=80.)
	2*	1-4	Alphanumeric code of first species whose initial concentration is to be reset (left-justified)
		11-14	Alphanumeric code of second species whose initial concentration is to be reset (left-justified)
		. . .	
		61-64	Alphanumeric code of seventh species whose initial concentration is to be reset (left-justified)
	3*	1-10	Concentration for first species (ppmV)
		11-20	Concentration for second species (ppmV)
		. . .	
		61-70	Concentration for seventh species (ppmV)

---

*If additional entries are required, they are continued on an input record immediately following the one with the first set of entries, using the same format.

TABLE 4-1G
INPUT FORMAT FOR ACCURACY OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
ACCURACY	Increase or reduce the mathematical accuracy of an isopleth diagram by using more or fewer simulations, more or less accurate interpolation, etc.		
	1	1-4	ACCU
		11-20	Number of constant initial $NMOC/NO_x$ ratios (radial lines emanating from the origin of the isopleth diagram) on which simulations are to be performed, any odd number from 1. to 19.; DF=11.
		21-30	Number of simulations per radial line, from 1. to 8.; DF=5.
		31-40	Error tolerance in the numerical integration routine, from 0.1 to 0.00001; DF=0.01
		41-50	Tension factor for hyperbolic spline functions used in first stage of interpolation from .001 to 50.; DF=1.
		51-60	Tension factor for hyperbolic spline functions used in plotting isopleth lines from .001 to 50.; DF=1.
		61-70	If any non-zero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces full length simulations

TABLE 4-1H
INPUT FORMAT FOR ALREADY OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
ALREADY			Include results from a previous run
	1	1- 4	ALRE
		11-20	Number of previous simulations to be input
	2*	1-10	Initial NMOC concentration, ppmC
		11-20	Initial NO_x concentration, ppm
		21-30	Maximum one-hour average ozone concentration, ppm

---

*One record is included for each simulation result. Thus, the number of these records must be equal to the value coded in columns 11-20 of Card 1. Also, the records must be put in the same order in which the simulations were performed.

TABLE 4-11
INPUT FORMAT FOR PLACE OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
PLACE			Input city-specific information on light intensity. Default values correspond to Los Angeles on June 21, 1975.
	1	1- 4	PLAC
		11-20	Latitude, in decimal degrees north of the equator; DF=34.058
		21-30	Longitude, in decimal degrees west of Greenwich meridian; DF=118.250
		31-40	The time zone, in hours from Greenwich mean time; DF=8.0
		41-50	The year; DF=1975.
		51-60	The month of year; DF=6.
		61-70	The numerical day of month; DF=21.
	2 (optional)	1-24	The name of the place can be entered anywhere in columns 1-24. Include this record only if a new value is entered for the latitude or longitude on the previous record

TABLE 4-1J
INPUT FORMAT FOR DILUTION OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
DILUTION			Input city-specific information on mixing heights
	1	1- 4	DILU
		11-20	Initial mixing height, in any units; DF=510.
		21-30	Final mixing height in same units as initial mixing height; DF=630.
		31-40	Starting time of rise in mixing height (24 hour daylight time); DF=800.
		41-50	Ending time of rise in mixing height (24 hour daylight time); DF= time corresponding to 70% of daylight hours

TABLE 4-1K
INPUT FORMAT FOR MIXING OPTION

OPTION		DESCRIPTION	
	RECORD NO.	COLUMNS	CONTENTS
MIXING		Used to supply hourly mixing heights for dilution	
	1	1- 4	MIXI
		11-20	Number of hours of dilution* (max = 15.)
		21-30	Mixing height at starting time of simulation, in any units
		31-40	Mixing height at end of first hour, in any units
		. . .	
		61-70	Mixing height at end of fourth hour, in any units
	2** (optional)	1-10	Mixing height at end of fifth hour, in any units
		. . .	
		61-70	Mixing height at end of eleventh hour, in any units
	3*** (optional)	1-10	Mixing height at end of twelfth hour, in any units
		. . .	
		31-40	Mixing height at end of fifteenth hour, in any units

*If n hours of dilution are specified, then n+1 non-zero mixing heights must be input.

**Included only if more than 4 hours of dilution are specified.

***Included only if more than 11 hours of dilution are specifed.

TABLE 4-1L
INPUT FORMAT FOR REACTIVITY OPTION

OPTION		DESCRIPTION	
	RECORD NO.	COLUMNS	CONTENTS
REACTIVITY		Used to supply city-specific information on NO_2/NO_x ratio and organic reactivity	
	1	1- 4	REAC
		11-20	Number of "hydrocarbon" species in the mechanism if organic reactivity inputs are to be supplied
		21-30	NO_2/NO_x ratio (DF=.25)
		31-40	Number of "aldehyde" species in the mechanism if organic reactivity factor inputs are to be supplied
	2* (optional)	1-10	Carbon fraction for first "hydrocarbon" species
		11-20	Carbon fraction for second "hydrocarbon" species
		. . .	
		61-70	Carbon fraction for seventh "hydrocarbon"

*Included only if a non-zero entry is made in columns 11-20 of input record 1. If additional entries are required, they are continued on the next input record using the same format as record number 2. (Note also that order of hydrocarbon species must be the same as that used in "MECHANISM" inputs.)

TABLE 4-1L (continued)
INPUT FORMAT FOR REACTIVITY OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
REACTIVITY (Cont'd)	3*	1-10	Carbon fraction for first "aldehyde" species
		11-20	Carbon fraction for second "aldehyde" species
		. . .	
		31-40	Carbon fraction for fourth "aldehyde" species

---

* Included only if non-zero entry is made in columns 31-40 of input record 1. Order of "aldehyde" species must be the same as that used in MECHANISM inputs

TABLE 4-1M
INPUT FORMAT FOR EMISSIONS OPTION

OPTION		DESCRIPTION	
	RECORD NO.	COLUMNS	CONTENTS
EMISSIONS		Input city-specific information on post-0800 emissions	
	1	1- 4	EMIS
		11-20	The number of hours for which emission fractions are to be input, from 1.0 to 15.0; DF=0. This number should be coded as positive if the same fractions for NMOC and NO_x are to be used. It should be coded as negative if different fractions are to be used.
		21-30	NMOC or NMOC and NO_x emission fraction for hour 1; DF=0. If all NMOC fractions are to be set to zero, enter any negative number and skip to record 3.
		31-40	NMOC or NMOC and NO_x emission fraction for hour 2; DF=0.
		. . .	
		61-70	NMOC or NMOC and NO_x emission fraction for hour 5; DF=0.
	2* (optional)	1-10	NMOC or NMOC and NO_x emission fraction for hour 6

*Input record 2 is included only if more than five hours of emissions are specified in columns 11-20 of input record 1, and if the first emission fraction entry on input record 1 is positive. If additional entries are required to specify NMOC or NMOC and NO_x fractions, they are continued on an input record immediately following the one with the first set of entries, using the same format.

TABLE 4-1M (continued)
INPUT FORMAT FOR EMISSIONS OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
EMISSIONS (Cont'd)			
		11-20	NMOC or NMOC and NO_x emission fraction for hour 7
		. . .	
		61-70	NMOC or NMOC and NO_x emission fraction for hour 12
	3* (optional)	1-10	NO_x emission fraction for hour 1. If all NO_x fractions are set to zero, then any negative number should be entered, and no further entries are required
		11-20	NO_x emission fraction for hour 2
		. . .	
		61-70	NO_x emission fraction for hour 7
	4* (optional)	1-10	NO_x emission fraction for hour 8
		11-20	NO_x emission fraction for hour 9
		. . .	
		61-70	NO_x emission fraction for hour 14

---

*Records 3 and 4 are included whenever separate NMOC and NO_x fractions are to be specified (i.e., columns 11-20 of input record 1 contains a negative number). Record 4 is included only when the number of hours of emissions is greater than 7. If the number of hours is greater than 14, the additional entries are made in an input record immediately following record number 4, using the same format.

TABLE 4-1N
INPUT FORMAT FOR MASSEMISS OPTION

OPTION		DESCRIPTION	
	RECORD NO.	COLUMNS	CONTENTS
MASSEMISS		Used to supply mass emission densities through which post-0800 emission fractions are computed	
	1	1- 4	MASS
		11-20	Number of hours of emissions (max=15.)
		21-30	Initial NMOC concentration used to compute NMOC emission fractions, ppmC
		31-40	Initial NO_x concentration used to compute NO_x emission fractions, ppm
		41-50	Mixing height at start of simulation, in meters
	2*	1-10	VOC emission density for hour 1, kg/km^2
		11-20	VOC emission density for hour 2, kg/km^2
		. . .	
		61-70	VOC emission density for hour 7, kg/km^2
	3*	1-10	NO_x emission density for hour 1, kg/km^2

---

*Number of entries must equal the number of hours of emissions specified in column 11-20 of input record 1. If additional entries are required, they are continued on an input record immediately following the one with the first set of entries, using the same format.

TABLE 4-1N (continued)
INPUT FORMAT FOR MASSEMISS OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
MASSEMISS (Cont'd)		11-20	NO_x emission density for hour 2, kg/km^2
		. . .	
		61-70	NO_x emission density for hour 7, kg/km^2

TABLE 4-10
INPUT FORMAT FOR TRANSPORT OPTION

OPTION		DESCRIPTION	
	RECORD NO.	COLUMNS	CONTENTS
TRANSPORT		Used to supply city-specific information on pollutants transported into city from upwind areas	
	1	1- 4	TRAN
		11-20	Concentration of ozone transported in surface layer, in ppm; DF=0
		21-30	Concentration of ozone transported aloft, in ppm; DF=0
		31-40	If the DODGE mechanism is being used, the total concentration of NMOC transported in surface layer, in ppmC; DF=0. If another mechanism is being used and surface layer transport is to be specified, the number of "hydrocarbon" species is coded as a negative number.
		41-50	If the DODGE mechanism is being used, the total concentration of NMOC transported aloft in ppmC; DF=0. If another mechanism is being used and transport aloft is to be specified, the number of "hydrocarbon" species is coded as a negative number.
		51-60	Concentration of NO_x transported in surface layer, in ppm; DF=0.*

---

*NO_x transport is assumed to be all NO_2.

TABLE 4-10 (continued)
INPUT FORMAT FOR TRANSPORT OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
TRANSPORT (Cont'd)			
		61-70	Concentration of NO_x transported aloft, in ppm; DF=0.*
	2** (optional)	1-10	The total NMOC concentration transported in surface layer, ppmC
		11-20	Surface layer transport carbon fraction for first "hydrocarbon" species
		21-30	Surface layer transport carbon fraction for second "hydrocarbon" species
		. . .	
		61-70	Surface layer transport carbon fraction for sixth "hydrocarbon" species
	3*** (optional)	1-10	Surface layer transport carbon fraction for first "aldehyde" species

---

[*] NO_x transport is assumed to be all NO_2.

[**] Included only if a negative entry is made in columns 31-40 of input record 1. One additional input record is required if the mechanism contains more than six hydrocarbon species. Carbon fraction entries for "hydrocarbon" species must be in the same order as specified in the MECHANISM and REACTIVITY options.

[***] Included only if a negative entry is made in columns 31-40 of input record 1, and the number of "aldehydes" in the mechanism is greater than zero.

TABLE 4-10 (continued)
INPUT FORMAT FOR TRANSPORT OPTION

OPTION	DESCRIPTION		
	RECORD NO.	COLUMNS	CONTENTS
TRANSPORT (Cont'd)			
		11-20	Surface layer transport carbon fraction for second "aldehyde" species
		. . .	
		31-40	Surface layer transport carbon fraction for fourth "aldehyde" species
	4* (optional)	1-10	The total NMOC concentration transported aloft, ppmC
		11-20	Aloft carbon fraction for first "hydrocarbon" species
		21-30	Aloft carbon fraction for second "hydrocarbon" species
		. . .	
		61-70	Aloft carbon fraction for sixth "hydrocarbon" species
	5** (optional)	1-10	Aloft carbon fraction for first "aldehyde" species
		11-20	Aloft carbon fraction for second "aldehyde" species
		. . .	
		34-40	Aloft carbon fraction for fourth "aldehyde" species

*Included only if a negative entry is made in columns 41-50 of input record 1. One additional input record is required if the mechanism contains more than six hydrocarbon species. Carbon fraction entries for "hydrocarbon" species must be in the same order as specified in the MECHANISM and REACTIVITY options.

**Included only if a negative entry is made in columns 41-50 of input record 1, and the number of "aldehydes" in the mechanism is greater than zero.

TABLE 4-1P
INPUT FORMAT FOR CALCULATE OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
CALCULATE			Perform a single simulation with the initial NMOC and NO_x concentrations specified on this record
	1	1- 4	CALC
		11-20	Initial NMOC concentration, in ppmC
		21-30	Initial NO_x concentration, in ppm
		31-40	Information option; entry of any positive value will result in printing of the computed concentrations of all species, the rates of change of all species, reaction rates, and photolysis rates.
		41-50	Time (in minutes) from the beginning of the simulation at which computed concentrations of all species in the kinetic mechanism are to be printed; DF=60.
		51-60	Time step (in minutes) for subsequent printing of concentrations; DF=60.

TABLE 4-1Q
INPUT FORMAT FOR ISOPLETH OPTION

OPTION	RECORD NO.	COLUMNS	CONTENTS
ISOPLETH			Construct an isopleth diagram according to the input parameters. Default isopleths are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36, and 0.40 ppm
	1	1- 4	ISOP
		11-20	Maximum NMOC concentration (in ppmC) on abscissa of isopleth diagram; DF=2.0
		21-30	Maximum NO_x concentration (in ppm) on ordinate of isopleth diagram; DF=0.28
		31-40	Number of isopleths to be drawn, from 1. to 20.; DF=11.
		41-50	Any non-zero value will activate the printing of solar noon and the time of the center of the maximum one-hour average concentration for each simulation
	2* (optional)	1-10	Concentration of 1st isopleth, ppm
		11-20	Concentration of 2nd isopleth, ppm
		. . .	
		61-70	Concentration of 7th isopleth, ppm

*Record number 2 is required only if an entry is made in columns 31-40 of input record 1 (i.e., isopleths to be specified). The number of entries in record 2 (and subsequent records) must equal the number of isopleths to be drawn, coded on input record 1. Additional entries are made on input records immediately following record number 2, using the same format.

TABLE 4-1R
INPUT FORMAT FOR EKMA OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
EKMA	Used to perform a VOC emission reaction calculation		
	1	1- 4	EKMA
		11-20	Base-case ozone concentration, ppm
		21-30	NMOC/NO_x ratio
		31-40	Percentage change in NO_x emissions; positive number for increase, negative number for decrease
		41-50	Change in transport option indicator; if non-zero, input record 2 is required
		51-60	Option to generate report of change in ozone as a function of change in VOC emissions; If 0., no report generated; If 1., generate tabular report; If 2., generate tabular report and write results to file.
	2* (optional)	1-10	Concentration of ozone transported in surface layer for post-control conditions, ppm; (DF = base-case level)

*Record number 2 is included only if non-zero entry is made in columns 41-50 of input record 1

TABLE 4-1R (continued)
INPUT FORMAT FOR EKMA OPTION

OPTION	DESCRIPTION RECORD NO.	COLUMNS	CONTENTS
EKMA (Cont'd)			
		11-20	Concentration of ozone transported aloft for post-control conditions, ppm; (DF = base case level)
		21-30	Concentration of NMOC transported in surface layer for post-control conditions, ppmC; (DF = base case level)
		31-40	Concentration of NMOC transported aloft for post-control conditions, ppmC; (DF = base case level)
		41-50	Concentration of NO_x transported in surface layer for post-control conditions, ppm; (DF = base case level)
		51-60	Concentration of NO_x transported aloft for post-control conditions, ppm; (DF = base case level)

Most options have specific, preset, default values associated with them, and these are noted in the tables. Any option may be omitted from the inputs whenever all of the defaults associated with that option are acceptable. Similarly, entries only need to be made in a particular field when it is desired to change a preset default (i.e., fields associated with a particular default-value that is acceptable may be left blank). Examples illustrating these coding conventions are contained in Chapter 5.

As noted earlier, the order that the option records are placed is not usually critical, so long as input data options precede functional options (i.e., the CALCULATE, ISOPLETH and EKMA options). Nevertheless, the order described in Section 3.3 is generally recommended. Any option included in an input data set will override a similar option previously specified. Thus, for example, if the DILUTION option is followed by the MIXING option, the MIXING option will be invoked. The MECHANISM and PLOT options, however, cannot be de-activated once invoked. Finally, the last input record of any set must be a blank record.

4.2 PROGRAM GENERATED MESSAGES

Two types of error messages can occur when executing OZIPM-2. First, fatal error messages are caused by problems that immediately halt program execution. Second, warnings may be produced by the program, although execution continues. Each are discussed below.

4.2.1 Fatal Error Messages

Nine fatal error messages may occur during OZIPM-2 model runs. Two are associated with the generation of ozone isopleth diagrams, five may result from problems encountered in the numerical integration and two others may occur with the SPECIES and MASSEMISS options. Each are described below, along with suggestions for corrective action.

ISOPLETH DIAGRAM MESSAGES:

- THE LOWEST _____ LINE CANNOT BE PLOTTED

  INCREASE THE MAXIMUM HC AND NO_x VALUES

  This message occurs when the species concentration predicted using the maximum initial NMOC and NO_x values is less than the lowest isopleth to be plotted. The problem may be corrected by enlarging the diagram (i.e., increasing the maximum initial NMOC and NO_x), or by reducing the concentrations of the isopleths that are requested.

- NO LINES CAN BE PLOTTED

  BACKGROUND ONLY PRODUCES TOO MUCH ___ ___ PPM

  This message occurs when the concentration predicted for the origin of the diagram (i.e., at NMOC and NO_x concentrations of zero) is greater than the highest isopleth to be plotted. If this message occurs, the NMOC, NO_x and ozone values entered with the TRANSPORT option should be checked for reasonableness. If a diagram for a species other than ozone is being produced, the concentrations of the isopleths requested may be increased.

NUMERICAL INTEGRATION MESSAGES:

- PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT

- INTEGRATION HALTED BY DRIVER AT T =

  EPS TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION

- KFLAG = -2 FROM INTEGRATOR AT T = _____, H = _____

  THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED

- KFLAG = -3 FROM INTEGRATOR AT T = _____

  CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED

- ILLEGAL INPUT..EPS.LE.O.

Should any of these error messages occur, the following steps are suggested.

1. Check to be sure that all input data are correct (e.g., check NMOC and NO_x concentrations entered on the CALCULATE option input record, check for inappropriate negative inputs, etc.).

2. If generating an isopleth diagram, redefine the density of simulations (e.g., change the diagram scales, change the number of radials, number of simulation points per line, etc.).

3. Increase the error tolerance.

4. As a last resort, alter the simulation conditions slightly (i.e., change post-0800 emissions, dilution, etc.).

SPECIES AND MASSEMISS MESSAGES:

- SPECIES _____ IS NOT FOUND IN THE KINETIC MECHANISM

  This message occurs when the SPECIES option is used, but the entry for the species does not match any in the mechanism. The SPECIES option inputs must be corrected (e.g., correct the alpha numeric code of the species, making sure it is left-justified).

- ERROR IN INPUT DATA FOR OPTION MASSEMISS

  This message occurs when the initial NMOC, initial NO_x, or initial mixing height input data on the MASSEMISS input record are not permissible values. Positive, non-zero entries are required for these variables.

4.2.2 Warning Messages

Warning messages may occur in the processing of the OZIPM-2 options and their associated inputs, or may occur when an isopleth diagram is being generated. Program execution is not halted by these types of messages, but corrective action may be required in some cases.

- THE OPTIONS INSTRUCTION _____ CANNOT BE PROCESSED

  This message occurs when an improper code is used for an option. The options should be checked to insure that the proper codes have been used, and that the numerical data required by the options in subsequent input records are present, and in the proper order.

- DUE TO HIGH BACKGROUND CONDITIONS

  THE LOWEST _____ PLOTTED WILL BE _____ PPM

  This message indicates that one or more of the lower isopleths lie too far to the left on the diagram to be plotted. For example, if background conditions were such that the predicted ozone concentration at the diagram origin was greater than 0.08 ppm, then the 0.08 ppm ozone isopleth could not be plotted, but isopleths corresponding to higher concentrations could possibly be drawn. Although no corrective action is required, the user may wish to check the TRANSPORT option inputs to insure that they are reasonable.

4.3 COMPUTER CONSIDERATIONS

The OZIPM-2 program consists of one main program and 47 subroutines written in FORTRAN. Every effort has been made to make the program as portable as possible. Nevertheless, some system incompatibilities inevitably arise, and some of the major ones are discussed below. Also included are discussions of computer resource requirements, input/output operations and the use of the CALCOMP subroutines. The final section contains example job control language.

A complete listing of the program is contained in the final appendix of this document. For reference, each subroutine has been assigned a letter code (e.g., A for MAIN), and each line within a subroutine has been numbered sequentially. Thus, reference to line A 5 refers to line number 5 of the MAIN program (i.e., A). These identifiers are located in columns 73 through 80 in the listing.

4.3.1 Potential System Incompatibilities

Although OZIPM-2 has been written to conform to ANSI FORTRAN, some language usage may not be compatible with all computer systems. Some of the identified incompatibilities are discussed below.

In subroutine SOLAR, two calls are made to the standard FORTRAN function for computing arcsin. As coded, the arcsin call is made using the function ASIN. On some computer systems, this function is referenced by a call to ARSIN. Lines D 61 and D 81 of subroutine SOLAR must be modified accordingly should this be the case.

Three of the subroutines in OZIPM-2 have multiple entry points:

SUBROUTINE DIFFUN	L 1
:	
ENTRY DIFSET	L 176
SUBROUTINE ISOPLT	V 1
:	
ENTRY SAVLIN	V 87
:	
ENTRY LINPRNT	V 108
SUBROUTINE VVLBLF	AS 1
:	
ENTRY VVLBLC	AS 60
:	
ENTRY VVLBLL	AS 165

Some reprogramming may be required if multiple entry points are not permitted.

As a natural occurrence of the numerical integration scheme used in OZIPM-2, underflows may result. (The latter can result from dividing a very small number by a large one or multiplying two very small numbers.) When this occurs, the proper corrective action is to set the resultant value to zero and continue with the calculations. Most computer systems have standard procedures for handling this situation. For example, with the UNIVAC-1100, this corrective action is taken automatically and no error message is generated. On some computer systems, however, it may be necessary to invoke special error handling routines and/or suppress the printing of any error messages associated with the occurrence of an underflow.

Two variables in OZIPM-2 must be set by the user to correspond to the computational characteristics of the specific computer that is to be used. These variables, UROUND and EXPMAX, are contained in the BLOCK DATA subroutine at lines AV 437 and AV 438, respectively. The preset values of these variables were selected for use with a UNIVAC 1100 computing system, but may require alteration when using another system.

The value of UROUND should be chosen such that it is slightly larger than the smallest number which gives a result different from one when it is added to one (i.e., 1.0 + UROUND should give a result greater than one). For the UNIVAC, an appropriate value is 7.5E-09, and for 32-bit machines such as IBM, 0.5E-06 is appropriate. For other systems, the value of UROUND may be calculated from the number of significant digits (N) used for the mantissa of a floating point number:

$$\mathrm{UROUND} = 2^{-N} \qquad (4\text{-}1)$$

Alternatively, it can be determined by trial and error from the condition that:

$$1.0 + \mathrm{UROUND} \neq 1$$

where UROUND is the smallest such positive number that satisfies the inequality. In practice, the value of UROUND that is used in OZIPM-2 can be slightly larger than the smallest value. If this number is set too small, the numerical integration routine will not find a solution, eventually aborting because of time limitations.

EXPMAX is set to insure that the maximum permissible value for the exponent of e is never exceeded, and is again machine dependent. The value of EXPMAX preset in OZIPM-2 is 87.4, which is slightly lower than the maximum permissible on a UNIVAC 1100. For an IBM system, a value of 174.0 is appropriate. The value of EXPMAX can be derived for other systems using the following relationship:

$$e^{\mathrm{EXPMAX}} = 10^{N} \qquad (4\text{-}2)$$

where 10^N is the largest value permitted for a real constant. EXPMAX should be set slightly lower than the number calculated, however. For example, EXPMAX calculated from equation 4-2 for the UNIVAC 1100 is 87.498, but was set to 87.4 to insure that this value is never reached.

4.3.2 Computer Requirements

The OZIPM-2 program requires approximately 65k words of storage on the UNIVAC 1100 computing system (i.e., 36-bit words). The only peripheral devices that may be required are mass-storage (or tape) files for the CALCOMP plot option and the EKMA generated file. These are discussed in subsequent sections of this chapter. The time requirements associated with OZIPM-2 runs will vary with computing system, and with the operations performed in the program. Nevertheless, the following approximate run times required on the UNIVAC computer system may prove useful:

Program Operation	Time Required
one CALCULATE	< 30 seconds
one EKMA	1 1/2 minutes
one ISOPLETH	5 minutes

The time required for multiple program operations within the same run can be approximated by adding the times for the individual runs.

4.3.3 Input/Output

The OZIPM-2 program is designed to read card-image input records (unit number 5) and produce line-printer output (unit number 6). These default unit assignments may be changed by modifying the variables IN and IOUT in the BLOCK DATA subroutine (lines AV 435 and AV 411), respectively. If an off-line plot is to be generated, OZIPM-2 produces CALCOMP compatible output on unit number 14. This unit can be changed by modifying line T 37 of subroutine LINER. Routing of the file to the off-line plotter is system dependent, and this must be handled on a case-by-case basis.

One option of the OZIPM-2 program is the generation of a file containing information produced by the EKMA routine (see Section 3.2.3.3). Output generated by this routine is written to a file on unit number 11. (Note that this file needs to be assigned only when this option is invoked, and the unit number can be changed in line number AE 15 of subroutine RANGE.) The output produced is card-image format (i.e., 80 columns), with one record generated per call to the EKMA option. The output consists of the ozone concentrations (F5.3 format) corresponding to base-conditions and to changes in VOC emissions. Thus, the record format is as follows:

Field Number	Columns	Contents
1	1- 5	Base-case ozone, ppm
2	6-10	Ozone predicted for a 10% VOC emission reduction, ppm
3	11-15	Ozone predicted for a 20% VOC emission reduction, ppm
	.	
	.	
	.	
11	51-55	Ozone predicted for a 100% VOC emission reduction, ppm

4.3.4 CALCOMP Routines

The CALCOMP routines used in OZIPM-2 include the following subroutines: PLOTS, PLOT, SYMBOL, NUMBER, and NEWPEN. Although these routines are only called when the PLOT option is included, user's without access to these systems subroutines may not be able to execute the program without explicitly linking them with the OZIPM-2 subroutines. This problem may be circumvented by creating a series of dummy subroutines with the aforementioned names as follows:

```
SUBROUTINE ____________ (argument list)

RETURN

END
```

For users with access to CALCOMP routines, the names of the subroutine calls used in OZIPM should be checked for consistency with system defined names, and the proper job control language should be used to link the system subroutines to OZIPM when generating an executable module.

4.3.5 Job Control Language

The following runstream illustrates the executive control language (ECL) necessary to execute the OZIPM-2 program on a UNIVAC 1100 computer system:

```
@RUN
@ASG,A     prog-file.
@PLOT      plotfile.
@XQT       prog-file.abs
INPUT RECORDS
@FREE      plotfile.
@SYM       plotfile.,,PLOT
@FIN
```

Although the job control language will be different for most computer systems, the fundamental requirements for executing OZIPM-2 on different systems are the same. The @RUN statement initiates the program run. The @ASG statement assigns the file containing the OZIPM-2 executable module (i.e., the absolute element in UNIVAC notation, the load module in IBM notation). A file that is to contain the data for CALCOMP plotting is assigned with the @PLOT statement. The @XQT statement initiates program execution, with the input data contained on the input records. The @FREE and @SYM statements route the CALCOMP produced file to the CALCOMP plotter for generation of the off-line PLOT. Finally, the @FIN signifies the end of the runstream. Note that if a CALCOMP plot is not desired, then the @PLOT, @FREE, and @SYM statements are omitted.

5.0 EXAMPLE OZIPM-2 RUNS

This chapter includes examples demonstrating some routine applications of OZIPM-2. Most emphasis is placed on the new features, such as the EKMA routine and the use of an alternate chemical mechanism. The user may also wish to review the examples contained in the OZIPP User's Manual, since many are relevant to the use of OZIPM-2 as well.

5.1 BENCHMARK EXAMPLE

When dealing with a program as complex as OZIPM-2, special care should be taken to insure that it is operating properly. Although almost any example run could serve as a benchmark, the approach taken here is to start with a simple example requiring minimal input data and minimal computer time. Before proceeding to the more complex examples, replication of the example shown in this section is recommended.

The input data set required for the first example is shown in Table 5-1. Only two input records are needed, one activating the CALCULATE option and the second (a blank record) indicating the end of the input data. The 1.0 and 0.10 on the CALCULATE option are the initial NMOC and NO_x concentrations. Calling the CALCULATE option in this manner causes the program to perform a single simulation with these levels using default values for all other model input variables.

The output for the example is shown in Figure 5-1, and can be broken down into three major parts. The first is a report summarizing the values of the city-specific model variables used in the simulation. The next portion consists of a table showing instantaneous pollutant concentrations at hourly intervals,

```
              1         2         3         4         5         6         7         8
     12345678901234567890123456789012345678901234567890123456789012345678901234567890

1    CALC      1.0       .10
2

     12345678901234567890123456789012345678901234567890123456789012345678901234567890
              1         2         3         4         5         6         7         8
```

TABLE 5-1. INPUT DATA FOR EXAMPLE 5-1

```
STANDARD OZONE ISOPLETH CONDITIONS


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR


          LOS ANGELES, CALIF.

LATITUDE      34.058

LONGITUDE     118.250

TIME ZONE     8.0

DATE          6     21    1975

TIME          800   TO    1800      LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS      INITIAL    510.     FINAL       630.

TIMING                 START      800.     STOP        1617.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME        800    900    1000   1100   1200   1300   1400   1500   1600   1700

HEIGHT    510.0  529.6  554.3  577.5  594.6  606.7  615.6  622.6  628.4  630.0



INITIAL          PROP FRACTION  .250   BUT   FRACTION  .750

INITIAL          HCHO FRACTION  .020   ALD2 FRACTION  .030

NO2/NOX        .250
```

FIGURE 5-1. OUTPUT FOR EXAMPLE 5-1

```
                    STANDARD OZONE ISOPLETH CONDITIONS
 TIME      HC       PROPYLENE     ALDEHYDE      NOX          NO2         O3
(LDT )    TOTAL     FRACTION      FRACTION     TOTAL       FRACTION   (INSTANT)

 800.    1.00000      .25000        .05000     .10000       .25000      .00000

 900.     .85976      .19914        .12125     .08918       .74353      .04122

1000.     .68346      .12119        .19282     .06472       .89553      .14549

1100.     .59731      .07946        .20577     .04828       .91473      .19441

1200.     .51651      .04189        .19310     .03040       .92556      .23425

1300.     .46529      .02279        .16907     .01869       .93086      .25259

1400.     .43387      .01415        .14895     .01207       .93405      .25950

1500.     .39903      .00748        .12368     .00588       .93880      .26256

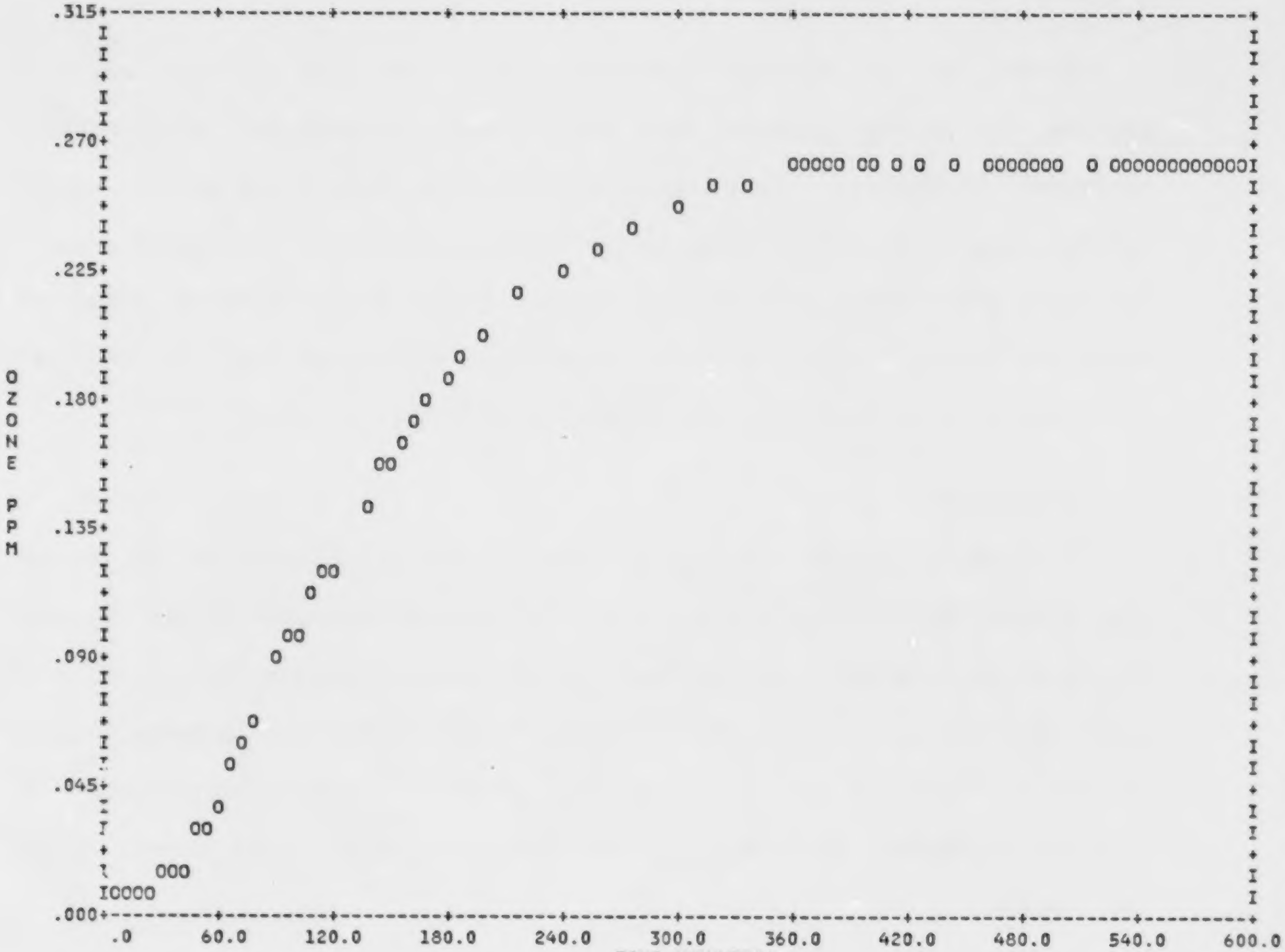
1600.     .36650      .00359        .09873     .00168       .94822      .26097

1700.     .35418      .00242        .08724     .00044       .95935      .26039

1800.     .34601      .00167        .07864     .00001       .97668      .25945

 MAXIMUM ONE HOUR AVE O3    =  .26245 CENTERED AT 434. MINUTES.
```

FIGURE 5-1. OUTPUT FOR EXAMPLE 5-1 (continued)



STANDARD OZONE ISOPLETH CONDITIONS

FIGURE 5-1. OUTPUT FOR EXAMPLE 5-1 (continued)

with the maximum one hour average concentration shown at the bottom of the table. The last page of output is a graph of instantaneous ozone concentration versus time.

Because of the internal precision associated with various computing systems, the outputs produced with two different systems may exhibit small numerical differences. Since most applications of OZIPM-2 are usually ozone-related, users may wish to focus on the ozone predictions. As a general rule, the ozone predictions shown in the tabular output should agree to about the third decimal place (i.e., 1 ppb). Substantial deviations (say, on the order of 10 ppb or more) could indicate program installation problems.

5.2 EKMA EXAMPLE

The example problem discussed in this section illustrates the use of the EKMA routine that is used to compute the VOC emission reduction needed to lower the base-case peak ozone concentration to the level of the standard (i.e., 0.12 ppm). To illustrate this application, a hypothetical set of city-specific data is used to establish the simulation conditions. A base-case ozone value of 0.22 ppm is assumed, and a base-case NMOC/NO_x ratio of 8.0 will be used in the calculations.

Table 5-2 shows the input data used in the example. The TITLE option is used to provide a title, and the PLACE option is used to define simulation light intensity through the specification of city-latitude (39°), city longitude (77°), time zone (5=EDT), year (1981), month (8), and day (1). The city name is located immediately following the PLAC option. The DILU, EMIS and TRAN options supply information on mixing heights, post-0800 emissions, and pollutant concentrations attributable to transport.

```
                 1         2         3         4         5         6         7         8
        12345678901234567890123456789012345678901234567890123456789012345678901234567890

 1      TITL
 2      EXAMPLE 5-2
 3      PLAC      39.       77.       5.        1981.     8.        1.
 4      CITY NAME
 5      DILU      250.      1500.
 6      EMIS      -8.0      .20       .20       .20       .10       .02
 7      .02       .02       .02
 8      .35       .35       .35       .20       .03       .03       .03
 9      .03
10      TRAN                .08
11      EKMA      .22       8.0       -5.0      1.0       1.0
12                .06
13

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                 1         2         3         4         5         6         7         8
```

TABLE 5-2. INPUT FOR EXAMPLE 5-2

First, the DILU record indicates that the initial mixing height is to be 250 meters, and the maximum afternoon mixing height is to be 1500 meters. The post-0800 emissions fractions are input with the EMIS option record, and the three subsequent record. Note that there are 8 hours of emissions in all. Finally, the TRAN record is used to set the level of ozone transported aloft to 0.08 ppm.

The EKMA input record contains information that is specifically required to perform the VOC emission reduction calculation. The first numeric field contains the base-case ozone concentration (0.22 ppm), and the second field contains the NMOC/NO_X ratio (8.0). The -5.0 in numeric field 3 indicates that NO_X emissions are expected to decrease by 5% between the base-case and the post-control case. The final two fields contain flags to activate two options within the EKMA routine. The 1.0 in the fourth numeric field indicates that a change in transport between the base-case and the post-control case is to be considered, and that an input record containing the post-control transport levels follows (i.e., the ozone aloft changes from 0.08 ppm in the base-case to 0.06 ppm in the post-control case in this example). The entry of 1.0 in the final field of the EKMA record causes the program to generate a tabular report showing ozone predictions as a function of VOC emission reductions. Note that since the MECHANISM option was not activated, the default DODGE mechanism is used in all calculations.

The output for this example is shown in Figure 5-2. The first portion simply summarizes the city-specific input information. The VOC emission reduction calculations are summarized in the table shown on page 129. Within this table, the input information on pollutant transport and assumed change in NO_X is first summarized. Then, the simulations conducted to find the base-case

```
EXAMPLE 5-2


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        CITY NAME

LATITUDE      39.000

LONGITUDE      77.000

TIME ZONE     5.0

DATE          8      1    1981

TIME          800   TO    1800      LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS       INITIAL   250.     FINAL      1500.

TIMING                  START     800.     STOP       1608.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME        800     900    1000    1100    1200    1300    1400    1500    1600    1700

HEIGHT    250.0   437.1   694.9   946.7  1134.1  1264.3  1358.4  1431.0  1492.2  1500.0



INITIAL          PROP FRACTION  .250   BUT  FRACTION  .750

INITIAL          HCHO FRACTION  .020   ALD2 FRACTION  .030

NO2/NOX        .250


TRANSPORTED CONCENTRATIONS

ALOFT                    OZONE    .080      HYDROCARBON   .000    NOX      .000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTON OF INITIAL

NON-BACKGROUND HYDROCARBON CONCENTRATION EMITTED PER HOUR)

    HOUR         1      2      3      4      5      6      7      8

    FRACTION  .200   .200   .200   .100   .020   .020   .020   .020

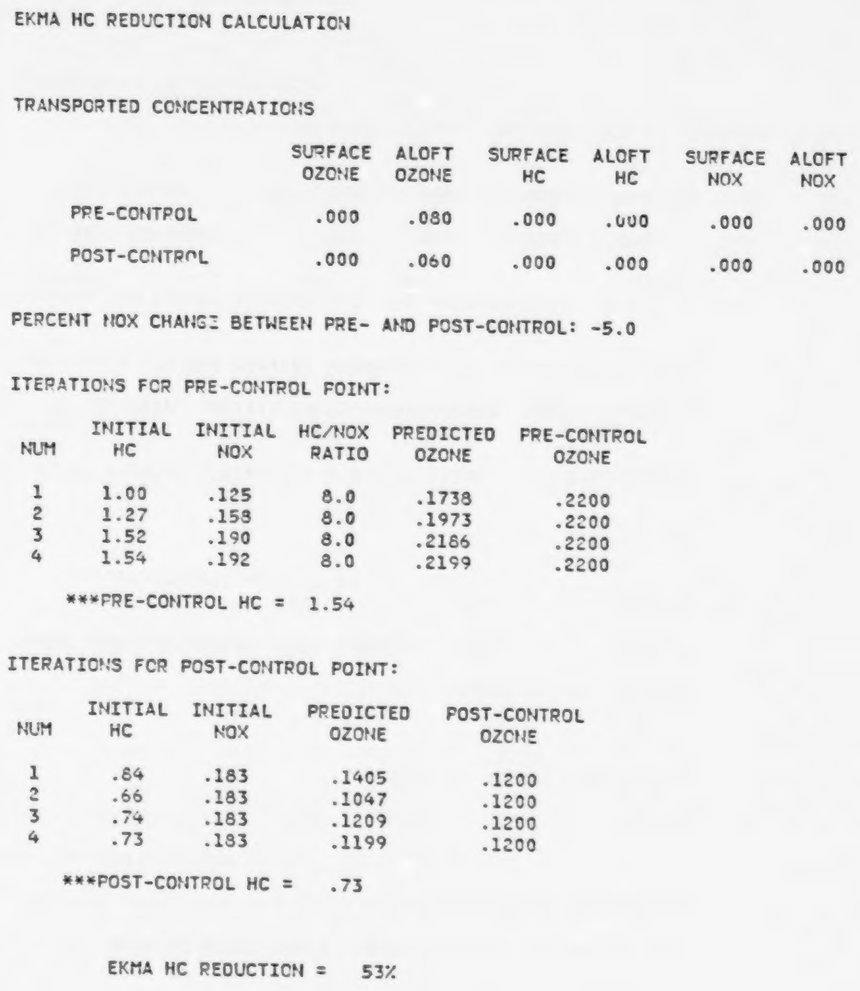

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF INITIAL

NON-BACKGROUND NOX CONCENTRATION EMITTED PER HOUR)

    HOUR         1      2      3      4      5      6      7      8

    FRACTION  .350   .350   .350   .200   .030   .030   .030   .030
```

FIGURE 5-2. OUTPUT FOR EXAMPLE 5-2



```
EKMA HC REDUCTION CALCULATION


TRANSPORTED CONCENTRATIONS

                            SURFACE  ALOFT   SURFACE  ALOFT   SURFACE  ALOFT
                             OZONE   OZONE     HC      HC       NOX     NOX

     PRE-CONTROL              .000    .080     .000    .000     .000    .000

     POST-CONTROL             .000    .060     .000    .000     .000    .000

PERCENT NOX CHANGE BETWEEN PRE- AND POST-CONTROL: -5.0

ITERATIONS FOR PRE-CONTROL POINT:

        INITIAL  INITIAL  HC/NOX  PREDICTED  PRE-CONTROL
 NUM      HC       NOX    RATIO     OZONE       OZONE

  1      1.00     .125     8.0      .1738       .2200
  2      1.27     .158     8.0      .1973       .2200
  3      1.52     .190     8.0      .2186       .2200
  4      1.54     .192     8.0      .2199       .2200

    ***PRE-CONTROL HC =  1.54

ITERATIONS FOR POST-CONTROL POINT:

        INITIAL  INITIAL   PREDICTED   POST-CONTROL
 NUM      HC       NOX       OZONE        OZONE

  1       .84     .183       .1405        .1200
  2       .66     .183       .1047        .1200
  3       .74     .183       .1209        .1200
  4       .73     .183       .1199        .1200

    ***POST-CONTROL HC =   .73


         EKMA HC REDUCTION =   53%
```

FIGURE 5-2. OUTPUT FOR EXAMPLE 5-2 (continued)

```
EKMA PREDICTED CHANGES IN OZONE


           HC      NOX      O3    %-CHG HC   %-CHG NOX   %-CHG O3

          1.540   .183   .2107         .0       -5.0        -4.2
          1.386   .183   .2013      -10.0       -5.0        -8.5
          1.232   .183   .1897      -20.0       -5.0       -13.8
          1.078   .183   .1745      -30.0       -5.0       -20.7
           .924   .183   .1544      -40.0       -5.0       -29.8
           .770   .183   .1277      -50.0       -5.0       -42.0
           .616   .183   .0953      -60.0       -5.0       -56.7
           .462   .183   .0624      -70.0       -5.0       -71.7
           .308   .183   .0369      -80.0       -5.0       -83.2
           .154   .183   .0240      -90.0       -5.0       -89.1
           .000   .183   .0196     -100.0       -5.0       -91.1
```

FIGURE 5-2. OUTPUT FOR EXAMPLE 5-2 (continued)

point are summarized by showing the assumed initial NMOC and NO_x concentrations and the predicted ozone concentration associated with each. Note that the simulations continue until predicted ozone level is within $\pm$0.0005 ppm of the observed ozone. Similar information is shown for the iterations performed to locate the post-control NMOC point. Note that the NO_x concentration used in these simulations was held constant for all iterations, and was calculated from the base-case NO_x concentration and the input percent change in NO_x. The simulations were continued until the predicted ozone level was within $\pm$0.0005 ppm of 0.12 ppm. Finally, the VOC reduction computation is summarized in the last line of the report by showing the pre-control NMOC point, the post-control NMOC point, and the resultant percent difference.

The final output table that is produced is the optional one showing predicted ozone concentrations as a function of change in VOC emissions. The table begins with the base case prediction, and then shows the predicted ozone concentration for incremental 10% reductions in VOCs, ranging from 10% to 100%. Note that the predicted ozone concentrations corresponding to each of the 11 cases (i.e., base case, 10% reduction...100% reduction) could be written to an output file if desired.

5.3 ALTERNATE MECHANISM EXAMPLE

The example in this section illustrates the use of a specific alternate chemical mechanism, the Carbon Bond 3 (CB-3) mechanism. Guidelines for using the CB-3 mechanism are contained in References 9 and 14, and the OZIPM-2 inputs were illustrated in Section 3.2.1.2 of this manual. The example problem presented here will show how the CB-3 mechanism is used with OZIPM-2 to generate an ozone isopleth diagram, following the recommended approach contained in

Reference 9. The city-specific information used in the previous example will also be used here.

The model inputs for the example problem are shown in Table 5-3. Record numbers 1 through 87 contain the CB-3 mechanism inputs. Since they were described in Section 3.2.1.2., the description will not be repeated here. Except for the REAC and TRAN options, the city-specific inputs are identical to those described in the previous section. The REAC option contains the input organic reactivity apportionment factors (i.e., carbon fractions). In this example, the default values recommended in Reference 9 have been used. Thus, 58% of NMOC is assumed to be PAR, 4% ETH, 3% OLE, etc. The TRAN option is used to supply information on pollutant concentrations transported in the surface layer and aloft. In the example, the ozone surface layer and aloft transport concentrations are 0.01 ppm, and 0.08 ppm, respectively. The next two fields, contain entries of "-7.0" that indicate that surface layer and aloft transport of NMOC are both to be considered. (Note that the number 7 actually refers to the total number of "hydrocarbon" species in the mechanism.) The input data associated with NMOC transport are provided on the next 4 input records. The first two records contain the surface layer transport information, and the next two contain the aloft information. In the example problem, the total NMOC concentration transported in the surface layer is assumed to be 0.038 ppmC, with 53% as PAR, 5% as ETH, 3% as OLE, etc. For transport aloft, the total NMOC concentration is 0.040 ppmC, with 61% as PAR, 6% as ETH, 3% as OLE, etc. The next to last input record, ISOP, directs OZIPM-2 to generate an isopleth diagram, and the blank record at the end signifies no further options are to be processed.

The output generated by the example problem is contained in Figure 5-3. As always, the first portion summarizes the city-specific inputs. Note also,

```
                 1         2         3         4         5         6         7         8
        12345678901234567890123456789012345678901234567890123456789012345678901234567890

 1      MECH      99.       7.0       7.0                           1.0
 2      1.        71.       99.       73.       38.       37.       67.
 3      67.
 4      PAR       ETH       OLE       ARO       HCHO      ALD2      NR
 5      1.        2.        2.        6.        1.        3.        1.
 6      NO2                1      NO      O                        1.00E+0
 7      O                  2      O3                               4.40E+6
 8      O3    NO           3      NO2                              2.66E+1 1450.0
 9      O3    NO2          4      NO3                               4.8E-2 2450.0
10      O     NO2          5      NO                               1.30E+4
11      O3    OH           6      HO2                               1.0E+2 1000.
12      O3    HO2          7      OH                                2.4E+0 1525.0
13      NO2   OH           8                                        1.6E+4
14      CO    OH           9      HO2                               4.4E+2
15      NO    NO          10      NO2     NO2                      1.50E-4
16      NO3   NO          11      NO2     NO2                       2.8E+4
17      NO3   NO2         12                                        2.6E+1 -10600.
18      HO2   NO          13      NO2     OH                        1.2E+4
19      HO2   HO2         14                                        1.5E+4
20      PAR   X           15                                        1.0E+5
21      PAR   OH          16      MEO2                              1.2E+3 560.0
22      OLE   O           17      MEO2    ACO3    X                 2.7E+3 325.0
23      OLE   O           18      HCHO    PAR                       2.7E+3 325.0
24      OLE   OH          19      RAO2                              3.7E+4 -540.0
25      OLE   O3          20      HCHO    CRIG                      8.0E-3 1900.0
26      OLE   O3          21      HCHO    MCRG    X                 8.0E-3 1900.0
27      ETH   O           22      MEO2    HO2     CO                6.0E+2 800.0
28      ETH   O           23      HCHO    PAR                       6.0E+2 800.0
29      ETH   OH          24      REO2                              1.2E+4 -332.0
30      ETH   O3          25      HCHO    CRIG                      2.4E-3 2560.0
31      ACO3  NO          26      NO2     MEO2                     1.04E+4
32      REO2  NO          27      NO2     HO2     HCHO    HCHO      1.2E+4
33      RAO2  NO          28      NO2     HO2     HCHO    HCHO      1.2E+4
34      MEO2  NO          29      NO2     MEO2    HCHO    X        3.70E+3
35      MEO2  NO          30      NO2     HCHO    HO2              7.40E+3
36      MEO2  NO          31                                        9.0E+2
37      REO2  O3          32      HCHO    HCHO    HO2               5.0E+0
38      RAO2  O3          33      HCHO    HCHO    HO2               2.0E+1
39      OH    HCHO        34      CRO2    X                         1.0E+2
40      HCHO  OH          35      HO2     CO                        9.0E+3

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                 1         2         3         4         5         6         7         8
```

TABLE 5-3. INPUT FOR EXAMPLE 5-3

```
                 1         2         3         4         5         6         7         8
        12345678901234567890123456789012345678901234567890123456789012345678901234567890

41      HCHO  OH        36      X       ACO3                      8.2E+3
42      HCHO            37      CO                                2.4E-1
43      HCHO            38      QQ                               5.64E-1
44      QQ              81      HO2     HO2     CO              8.867E+3
45      QQ              82      MEO2    MEO2    X       XCO     1.133E+3
46      XCO             83      X       CO                        1.0E+4
47      ACO3  NO2       39      PAN                               7.0E+3
48      PAN             40      ACO3    NO2                       2.2E-2 13500.0
49      ACO3  HO2       41                                        1.5E+4
50      MEO2  HO2       42                                        9.0E+3
51      CRIG  NO        43      NO2     HCHO                      1.2E+4
52      CRIG  NO2       44      NO3     HCHO                      8.0E+3
53      CRIG  HCHO      45                                        2.0E+3
54      MCRG  NO        46      NO2     HCHO    PAR               1.2E+4
55      MCRG  NO2       47      NO3     HCHO    PAR               8.0E+3
56      MCRG  HCHO      48                                        2.0E+3
57      CRIG            49      CO                                6.7E+2
58      CRIG            50                                        2.4E+2
59      CRIG            51      HO2     HO2     CO                9.0E+1
60      MCRG            52                                        1.5E+2
61      MCRG            53      MEO2    OH      CO                3.4E+2
62      MCRG            54      MEO2    HO2                      4.25E+2
63      MCRG            55      HCHO    HO2     HO2     CO        8.5E+1
64      ARO   OH        56      RARO                              6.0E+3 600.0
65      ARO   OH        57      HO2     OPEN                     1.45E+4 400.0
66      RARO  NO        58      NO2     PHEN    HO2               4.0E+3
67      OPEN  NO        59      NO2     ALD2    X       AFRC      6.0E+3
68      AFRC            60      ALD2    HCHO    CO      X         1.0E+4
69      AFRC            61      HCHO    HCHO    CO      CO        1.0E+4
70      PHEN  NO3       62      PHO     HNO3                      5.0E+3
71      PHO   NO2       63                                        4.0E+3
72      PHO   HO2       64      PHEN                              5.0E+4
73      OPEN  O3        65      ALD2    X       AFRC              4.0E+1
74      OH    PHEN      66      HO2     AFRC    PAR     HCHO      3.0E+4
75      ALD2            67      HO2     ACO3    CO                2.0E-2
76      PHEN  OH        68      PHO                               1.0E+4
77      CRO2  NO        69      NO2     HCHO    ACO3    X         1.2E+4
78      ALD2  OH        70      ACO3    CO                        2.5E+4
79      HONO            71      OH      NO                         3.1E0
80      OH    NO        72      HONO                             9.77E+3

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                 1         2         3         4         5         6         7         8
```

TABLE 5-3. INPUT FOR EXAMPLE 5-3 (continued -2)

```
         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890


O3              73      O1D                               5.4E-1
O1D             74      O                               4.44E+10
O1D             75      OH      OH                        6.8E+9
OH              90      HO2                               8.8E+1
OH              91      MEO2                              2.8E+1
NR              92      NR                                1.0E+0
O3              99      O                                 1.0E+0
TITL
EXAMPLE 5-3
PLAC      39.       77.       5.        1981.     8.        1.
CITY NAME
DILU      250.      1500.
EMIS      -8.0      .20       .20       .20       .10       .02
.02       .02       .02
.35       .35       .35       .20       .03       .03       .03
.03
REAC      7.
.53       .04       .03       .19       .05       .00       .15
TRAN      .01       .08       -7.0      -7.0
.038      .53       .05       .03       .13       .26       .00
.00
.040      .61       .06       .03       .15       .15       .00
.00
ISOP


12345678901234567890123456789012345678901234567890123456789012345678901234567890
         1         2         3         4         5         6         7         8
```

TABLE 5-3. INPUT FOR EXAMPLE 5-3 (continued -3)

```
THE REACTIONS ARE

  1   NO2                  =          NO        O                                     1.000+000      .000
  2   O                    =          O3                                              4.400+006      .000
  3   O3        NO         =          NO2                                             2.660+001     1.450+0
  4   O3        NO2        =          NO3                                             4.800-002     2.450+0
  5   O         NO2        =          NO                                              1.300+004      .000
  6   O3        OH         =          HO2                                             1.000+002     1.000+0
  7   O3        HO2        =          OH                                              2.400+000     1.525+0
  8   NO2       OH         =                                                          1.600+004      .000
  9   CO        OH         =          HO2                                             4.400+002      .000
 10   NO        NO         =          NO2       NO2                                   1.500-004      .000
 11   NO3       NO         =          NO2       NO2                                   2.800+004      .000
 12   NO3       NO2        =                                                          2.600+001    -1.060+0
 13   HO2       NO         =          NO2       OH                                    1.200+004      .000
 14   HO2       HO2        =                                                          1.500+004      .000
 15   PAR       X          =                                                          1.000+005      .000
 16   PAR       OH         =          MEO2                                            1.200+003     5.600+0
 17   OLE       O          =          MEO2      ACO3                X                 2.700+003     3.250+0
 18   OLE       O          =          HCHO      PAR                                   2.700+003     3.250+0
 19   OLE       OH         =          RAO2                                            3.700+004    -5.400+0
 20   OLE       O3         =          HCHO      CRIG                                  8.000-003     1.900+0
 21   OLE       O3         =          HCHO      MCRG                X                 8.000-003     1.900+0
 22   ETH       O          =          MEO2      HO2                 CO                6.000+002     8.000+0
 23   ETH       O          =          HCHO      PAR                                   6.000+002     8.000+0
 24   ETH       OH         =          RBO2                                            1.200+004    -3.820+0
 25   ETH       O3         =          HCHO      CRIG                                  2.400-003     2.560+0
 26   ACO3      NO         =          NO2       MEO2                                  1.040+004      .000
 27   RBO2      NO         =          NO2       HO2                 HCHO      HCHO    1.200+004      .000
 28   RAO2      NO         =          NO2       HO2                 HCHO      HCHO    1.200+004      .000
 29   MEO2      NO         =          NO2       MEO2                HCHO      X       3.700+003      .000
 30   MEO2      NO         =          NO2       HCHO                HO2               7.400+003      .000
 31   MEO2      NO         =                                                          9.000+002      .000
 32   RBO2      O3         =          HCHO      HCHO                HO2               5.000+000      .000
 33   RAO2      O3         =          HCHO      HCHO                HO2               2.000+001      .000
 34   OH        HCHO       =          CRO2      X                                     1.000+002      .000
 35   HCHO      OH         =          HO2       CO                                    9.000+003      .000
 36   HCHO      OH         =          X         ACO3                                  8.200+003      .000
 37   HCHO                 =          CO                                              2.400-001      .000
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3

```
 38   HCHO               =      QQ                                  5.640-001     .000
 81   QQ                 =      HO2     HO2          CO             8.867+003     .000
 82   QQ                 =      MEO2    MEO2         X       XCO    1.133+003     .000
 83   XCO                =      X       CO                          1.000+004     .000
 39   ACO3     NO2       =      PAN                                 7.000+003     .000
 40   PAN                =      ACO3    NO2                         2.200-002    1.350+0
 41   ACO3     HO2       =                                          1.500+004     .000
 42   MEO2     HO2       =                                          9.000+003     .000
 43   CRIG     NO        =      NO2     HCHO                        1.200+004     .000
 44   CRIG     NO2       =      NO3     HCHO                        8.000+003     .000
 45   CRIG     HCHO      =                                          2.000+003     .000
 46   MCRG     NO        =      NO2     HCHO         PAR            1.200+004     .000
 47   MCRG     NO2       =      NO3     HCHO         PAR            8.000+003     .000
 48   MCRG     HCHO      =                                          2.000+003     .000
 49   CRIG               =      CO                                  6.700+002     .000
 50   CRIG               =                                          2.400+002     .000
 51   CRIG               =      HO2     HO2          CO             9.000+001     .000
 52   MCRG               =                                          1.500+002     .000
 53   MCRG               =      MEO2    OH           CO             3.400+002     .000
 54   MCRG               =      MEO2    HO2                         4.250+002     .000
 55   MCRG               =      HCHO    HO2          HO2     CO     8.500+001     .000
 56   ARO      OH        =      RARO                                6.000+003    6.000+0
 57   ARO      OH        =      HO2     OPEN                        1.450+004    4.000+0
 58   RARO     NO        =      NO2     PHEN         HO2            4.000+003     .000
 59   OPEN     NO        =      NO2     ALD2         X       APRC   6.000+003     .000
 60   APRC               =      ALD2    HCHO         CO      X      1.000+004     .000
 61   APRC               =      HCHO    HCHO         CO      CO     1.000+004     .000
 62   PHEN     NO3       =      PHO     HNO3                        5.000+003     .000
 63   PHO      NO2       =                                          4.000+003     .000
 64   PHO      HO2       =      PHEN                                5.000+004     .000
 65   OPEN     O3        =      ALD2    X            APRC           4.000+001     .000
 66   OH       PHEN      =      HO2     APRC         PAR     HCHO   3.000+004     .000
 67   ALD2               =      HO2     ACO3         CO             2.000-002     .000
 68   PHEN     OH        =      PHO                                 1.000+004     .000
 69   CRO2     NO        =      NO2     HCHO         ACO3    X      1.200+004     .000
 70   ALD2     OH        =      ACO3    CO                          2.500+004     .000
 71   HONO               =      OH      NO                          3.100+000     .000
 72   OH       NO        =      HONO                                9.770+003     .000
 73   O3                 =      O1D                                 5.400-001     .000
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)

```
74   O1D                    =       O                                        4.440+010     .000
75   O1D                    =       OH       OH                              6.800+009     .000
90   OH                     =       HO2                                      8.800+001     .000
91   OH                     =       MEO2                                     2.800+001     .000
92   NR                     =       NR                                       1.000+000     .000
99   O3                     =       O                                        1.000+000     .000
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)

```
EXAMPLE 5-3


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR


         CITY NAME


LATITUDE      39.000

LONGITUDE      77.000

TIME ZONE     5.0

DATE          8      1   1981

TIME          800    TO   1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS      INITIAL   250.     FINAL      1500.

TIMING                 START     800.     STOP       1608.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME        800    900   1000   1100   1200   1300   1400   1500   1600   1700


HEIGHT    250.0  437.1  694.9  946.7 1134.1 1264.3 1358.4 1431.0 1492.2 1500.0




INITIAL          PAR  FRACTION  .580   ETH  FRACTION  .040   OLE  FRACTION  .030

INITIAL          ARO  FRACTION  .190   HCHO FRACTION  .050   ALD2 FRACTION  .000

INITIAL          NR   FRACTION  .150

NO2/NOX         .250

THERE ARE NO ALDEHYDES IN THE MECHANISM


TRANSPORTED CONCENTRATIONS

SURFACE LAYER          OZONE     .010     HYDROCARBON   .038    NOX       .000 PPM

ALOFT                  OZONE     .080     HYDROCARBON   .040    NOX       .000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTON OF INITIAL

NON-BACKGROUND HYDROCARBON CONCENTRATION EMITTED PER HOUR)

     HOUR         1     2     3     4     5     6     7     8

     FRACTION  .200  .200  .200  .100  .020  .020  .020  .020


CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF INITIAL

NON-BACKGROUND NOX CONCENTRATION EMITTED PER HOUR)
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)

```
HOUR         1      2      3      4      5      6      7      8
FRACTION  .350   .350   .350   .200   .030   .030   .030   .030
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)

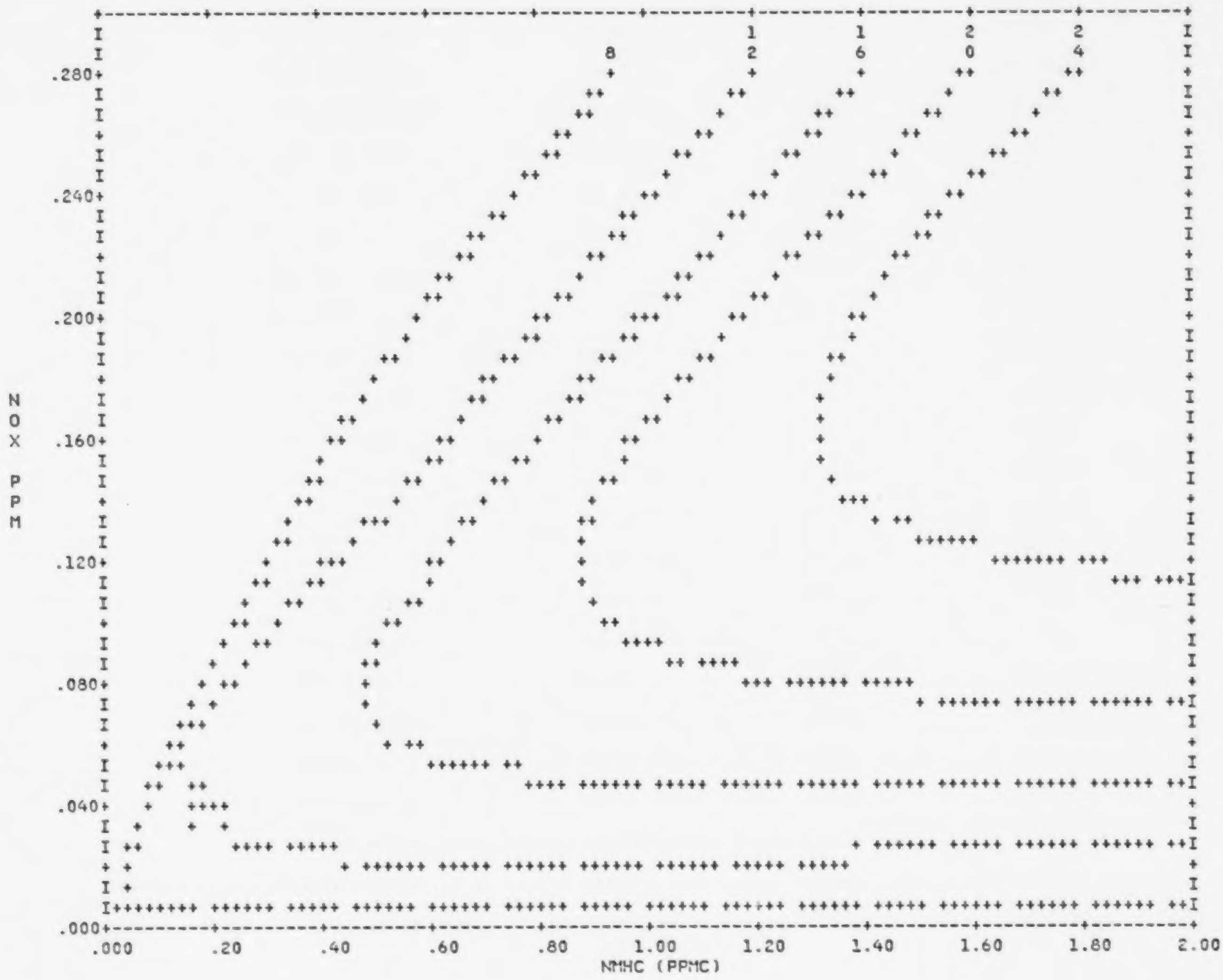
```
THE FOLLOWING SIMULATIONS WERE DONE.

     HC               NOX              RATIO             O3
   .00000           .00000            .00000           .06276
   .00000           .28000            .00000           .02147
  2.00000           .28000           7.14286           .27912 NOT MAX
  2.00000           .00000            .00000           .05889
   .85485           .28000           3.05305           .06849 NOT MAX
  2.00000           .02684          74.51248           .12933 NOT MAX
  1.30770           .18308           7.14286           .23600 NOT MAX
   .65385           .09154           7.14286           .17886 NOT MAX
   .32692           .04577           7.14286           .13830 NOT MAX
   .05182           .00726           7.14286           .08370 NOT MAX
  1.77685           .28000           6.34590           .23683 NOT MAX
  1.20236           .18947           6.34590           .21459 NOT MAX
   .72604           .11441           6.34590           .18539 NOT MAX
   .36302           .05721           6.34590           .14610 NOT MAX
   .05161           .00813           6.34590           .08553 NOT MAX
  1.47932           .28000           5.28330           .17419 NOT MAX
  1.07050           .20262           5.28330           .16996 NOT MAX
   .69351           .13126           5.28330           .16831 NOT MAX
   .35004           .06625           5.28330           .14690 NOT MAX
   .02338           .00442           5.28330           .07638 NOT MAX
  1.24988           .28000           4.46385           .12965 NOT MAX
   .97440           .21829           4.46385           .13188 NOT MAX
   .48720           .10914           4.46385           .14608 NOT MAX
   .24360           .05457           4.46385           .13458 NOT MAX
   .02084           .00467           4.46385           .07704 NOT MAX
  1.05919           .28000           3.78281           .09757 NOT MAX
   .84735           .22400           3.78281           .10284 NOT MAX
   .42368           .11200           3.78281           .12604 NOT MAX
   .21184           .05600           3.78281           .13096 NOT MAX
   .00726           .00192           3.78281           .06921
   .77745           .28000           2.77661           .05955 NOT MAX
   .38872           .14000           2.77661           .08769 NOT MAX
   .38638           .13915           2.77661           .08818 NOT MAX
   .31098           .11200           2.77661           .09840 NOT MAX
   .15042           .05418           2.77661           .12286 NOT MAX
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)

```
     2.00000              .23467           8.52246           .29618 NOT MAX
     1.29174              .15157           8.52246           .23777 NOT MAX
      .64587              .07578           8.52246           .17359 NOT MAX
      .32293              .03789           8.52246           .13283 NOT MAX
      .05654              .00663           8.52246           .08238 NOT MAX
     2.00000              .18935          10.56256           .28650 NOT MAX
     1.30064              .12314          10.56256           .22919 NOT MAX
      .65032              .06157          10.56256           .16604 NOT MAX
      .32516              .03078          10.56256           .12659 NOT MAX
      .06470              .00613          10.56256           .08129 NOT MAX
     2.00000              .14402          13.88675           .26309 NOT MAX
     1.32387              .09533          13.88675           .21335 NOT MAX
      .66193              .04767          13.88675           .15517 NOT MAX
      .33097              .02383          13.88675           .11848 NOT MAX
      .07895              .00569          13.88675           .08030 NOT MAX
     2.00000              .09870          20.26420           .22723 NOT MAX
     1.36527              .06737          20.26420           .18894 NOT MAX
      .72052              .03556          20.26420           .14238 NOT MAX
      .36026              .01778          20.26420           .10957 NOT MAX
      .10797              .00533          20.26420           .07947 NOT MAX
     2.00000              .05337          37.47405           .17290 NOT MAX
     1.44976              .03869          37.47405           .15103 NOT MAX
      .85047              .02269          37.47405           .12227 NOT MAX
      .43992              .01174          37.47405           .09761 NOT MAX
      .19194              .00512          37.47405           .07915 NOT MAX
      .73760              .28000           2.63429           .05512 NOT MAX
     2.00000              .00638         313.44209           .08194
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)



```
EXAMPLE 5-3

THE O3   LINES ARE    .08000  .12000  .16000  .20000  .24000
```

FIGURE 5-3. OUTPUT FOR EXAMPLE 5-3 (continued)

however, that the chemical mechanism is listed as well. The output generated by the ISOPLETH option consists of two parts. The first is a tabular report summarizing the simulations that were performed to generate the diagram. The second part is the line printer plot of the isopleth diagram itself.

5.4 MISCELLANEOUS OPTION EXAMPLE

The final example discussed in this section is included to illustrate several of the other new options in OZIPM-2 that were not used in the previous examples, specifically MIXING, MASSEMISS, TIME, INITIAL, and SPECIES. The city-specific data used in this example are structured around those used in the last example, and the CB-3 mechanism is also used. In this case, however, the SPECIES and ISOPLETH options will be used to generate an NO_2 isopleth diagram instead of an ozone isopleth diagram.

Table 5-4 contains the model inputs for the final example. In this example, the MIXING option has replaced the DILU option, and the hourly mixing height values used in the simulations are shown on the input records. Note that a total of 8 hours of dilution was considered, requiring that 9, hourly, mixing heights be specified. The MASSEMISS inputs include the information needed to compute the post-0800 emission fractions: number of hours of emissions (8), initial NMOC concentration (1.2 ppmC), initial NO_x concentration (0.150 ppm), and initial mixing height (250 meters). The emission densities of VOC and NO_x, in kg/km^2, are contained on the subsequent input records. The TIME option is used to increase the length of the simulation in this example by changing the ending time to 2000 hours LDT, instead of the default 1800. The INITIAL option can be used to establish the initial concentration of any species, and in the example the species selected is PAN (i.e., peroxyacetylnitrate), and its initial concentration is set to 0.005 ppm. Finally, the SPECIES option, located anywhere before the ISOPLETH option, causes the OZIPM-2 program to generate an isopleth diagram for the named species (NO_2), rather than for ozone.

Figure 5-4 includes the output obtained with the example input data. As always, the first portion lists the chemical mechanism and gives a summary of the city-specific model input data. As in the previous example, the next portion of the output is a tabular summary of the simulations that were performed to generate the isopleth diagram. In this example, maximum, 1 hour concentrations of NO_2, rather than O_3, are shown. Finally, the NO_2 isopleth diagram is the last of the ISOPLETH generated outputs.

```
                 1         2         3         4         5         6         7         8
        12345678901234567890123456789012345678901234567890123456789012345678901234567890

 1      MECH      99.       7.0       7.0                           1.0
 2      1.        71.       99.       73.       38.       37.       67.
 3      67.
 4      PAR       ETH       OLE       ARO       HCHO      ALD2      NR
 5      1.        2.        2.        6.        1.        3.        1.
 6      NO2              1      NO      O                         1.00E+0
 7      O                2      O3                                4.40E+6
 8      O3    NO         3      NO2                               2.66E+1 1450.0
 9      O3    NO2        4      NO3                                4.8E-2 2450.0
10      O     NO2        5      NO                                1.30E+4
11      O3    OH         6      HO2                                1.0E+2 1000.
12      O3    HO2        7      OH                                 2.4E+0 1525.0
13      NO2   OH         8                                         1.6E+4
14      CO    OH         9      HO2                                4.4E+2
15      NO    NO        10      NO2     NO2                       1.50E-4
16      NO3   NO        11      NO2     NO2                        2.8E+4
17      NO3   NO2       12                                         2.6E+1 -10600.
18      HO2   NO        13      NO2     OH                         1.2E+4
19      HO2   HO2       14                                         1.5E+4
20      PAR   X         15                                         1.0E+5
21      PAR   OH        16      MEO2                               1.2E+3 560.0
22      OLE   O         17      MEO2    ACO3    X                  2.7E+3 325.0
23      OLE   O         18      HCHO    PAR                        2.7E+3 325.0
24      OLE   OH        19      RAO2                               3.7E+4 -540.0
25      OLE   O3        20      HCHO    CRIG                       8.0E-3 1900.0
26      OLE   O3        21      HCHO    MCRG    X                  8.0E-3 1900.0
27      ETH   O         22      MEO2    HO2     CO                 6.0E+2 800.0
28      ETH   O         23      HCHO    PAR                        6.0E+2 800.0
29      ETH   OH        24      RBO2                               1.2E+4 -332.0
30      ETH   O3        25      HCHO    CRIG                       2.4E-3 2560.0
31      ACO3  NO        26      NO2     MEO2                      1.04E+4
32      RBO2  NO        27      NO2     HO2     HCHO    HCHO       1.2E+4
33      RAO2  NO        28      NO2     HO2     HCHO    HCHO       1.2E+4
34      MEO2  NO        29      NO2     MEO2    HCHO    X         3.70E+3
35      MEO2  NO        30      NO2     HCHO    HO2               7.40E+3
36      MEO2  NO        31                                         9.0E+2
37      RBO2  O3        32      HCHO    HCHO    HO2                5.0E+0
38      RAO2  O3        33      HCHO    HCHO    HO2                2.0E+1
39      OH    HCHO      34      CRO2    X                          1.0E+2
40      HCHO  OH        35      HO2     CO                         9.0E+3

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                 1         2         3         4         5         6         7         8
```

TABLE 5-4. INPUT FOR EXAMPLE 5-4

```
                1         2         3         4         5         6         7         8
       12345678901234567890123456789012345678901234567890123456789012345678901234567890

41     HCHO  OH        36      X       ACO3                       8.2E+3
42     HCHO            37      CO                                 2.4E-1
43     HCHO            38      QQ                                5.64E-1
44     QQ              81      HO2     HO2     CO               8.867E+3
45     QQ              82      MEO2    MEO2    X       XCO      1.133E+3
46     XCO             83      X       CO                         1.0E+4
47     ACO3  NO2       39      PAN                                7.0E+3
48     PAN             40      ACO3    NO2                        2.2E-2 13500.0
49     ACO3  HO2       41                                         1.5E+4
50     MEO2  HO2       42                                         9.0E+3
51     CRIG  NO        43      NO2     HCHO                       1.2E+4
52     CRIG  NO2       44      NO3     HCHO                       8.0E+3
53     CRIG  HCHO      45                                         2.0E+3
54     MCRG  NO        46      NO2     HCHO    PAR                1.2E+4
55     MCRG  NO2       47      NO3     HCHO    PAR                8.0E+3
56     MCRG  HCHO      48                                         2.0E+3
57     CRIG            49      CO                                 6.7E+2
58     CRIG            50                                         2.4E+2
59     CRIG            51      HO2     HO2     CO                 9.0E+1
60     MCRG            52                                         1.5E+2
61     MCRG            53      MEO2    OH      CO                 3.4E+2
62     MCRG            54      MEO2    HO2                       4.25E+2
63     MCRG            55      HCHO    HO2     HO2     CO         8.5E+1
64     ARO   OH        56      RARO                               6.0E+3 600.0
65     ARO   OH        57      HO2     OPEN                      1.45E+4 400.0
66     RARO  NO        58      NO2     PHEN    HO2                4.0E+3
67     OPEN  NO        59      NO2     ALD2    X       APRC       6.0E+3
68     APRC            60      ALD2    HCHO    CO      X          1.0E+4
69     APRC            61      HCHO    HCHO    CO      CO         1.0E+4
70     PHEN  NO3       62      PHO     HNO3                       5.0E+3
71     PHO   NO2       63                                         4.0E+3
72     PHO   HO2       64      PHEN                               5.0E+4
73     OPEN  O3        65      ALD2    X       APRC               4.0E+1
74     OH    PHEN      66      HO2     APRC    PAR     HCHO       3.0E+4
75     ALD2            67      HO2     ACO3    CO                 2.0E-2
76     PHEN  OH        68      PHO                                1.0E+4
77     CRO2  NO        69      NO2     HCHO    ACO3    X          1.2E+4
78     ALD2  OH        70      ACO3    CO                         2.5E+4
79     HONO            71      OH      NO                         3.1E0
80     OH    NO        72      HONO                              9.77E+3

       12345678901234567890123456789012345678901234567890123456789012345678901234567890
                1         2         3         4         5         6         7         8
```

TABLE 5-4. INPUT FOR EXAMPLE 5-4 (continued -2)

```
                 1         2         3         4         5         6         7         8
        12345678901234567890123456789012345678901234567890123456789012345678901234567890

 81     O3              73      O1D                                5.4E-1
 82     O1D             74      O                                4.44E+10
 83     O1D             75      OH      OH                         6.8E+9
 84     OH              90      HO2                                8.8E+1
 85     OH              91      MEO2                               2.8E+1
 86     NR              92      NR                                 1.0E+0
 87     O3              99      O                                  1.0E+0
 88     TITL
 89     EXAMPLE 5-4
 90     TIME      800.      2000.
 91     INIT      1.0
 92     PAN
 93     .005
 94     SPEC
 95     NO2
 96     PLAC      39.       77.       5.        1981.     8.        1.
 97     CITY NAME
 98     MIXI      8.0       250.      410.      620.      810.      950.
 99     1050.     1120.     1180.     1220.
100     MASS      8.        1.2       .150      250.
101     50.       50.       50.       25.       5.        5.        5.
102     5.
103     25.       25.       25.       15.       3.        3.        3.
104     3.
105     REAC      7.
106     .53       .04       .03       .19       .05       .00       .15
107     TRAN      .01       .08       -7.0      -7.0
108     .038      .53       .05       .03       .13       .26       .00
109     .00
110     .040      .61       .06       .03       .15       .15       .00
111     .00
112     ISOP                          7.0
113     .02       .04       .06       .08       .10       .12       .14
114

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                 1         2         3         4         5         6         7         8
```

TABLE 5-4. INPUT FOR EXAMPLE 5-4 (continued -3)

```
THE REACTIONS ARE

  1  NO2                 =       NO        O                                       1.000+000        .000
  2  O                   =       O3                                                4.400+006        .000
  3  O3        NO        =       NO2                                               2.660+001   1.450+003
  4  O3        NO2       =       NO3                                               4.800-002   2.450+003
  5  O         NO2       =       NO                                                1.300+004        .000
  6  O3        OH        =       HO2                                               1.000+002   1.000+003
  7  O3        HO2       =       OH                                                2.400+000   1.525+003
  8  NO2       OH        =                                                         1.600+004        .000
  9  CO        OH        =       HO2                                               4.400+002        .000
 10  NO        NO        =       NO2       NO2                                     1.500-004        .000
 11  NO3       NO        =       NO2       NO2                                     2.800+004        .000
 12  NO3       NO2       =                                                         2.600+001  -1.060+004
 13  HO2       NO        =       NO2       OH                                      1.200+004        .000
 14  HO2       HO2       =                                                         1.500+004        .000
 15  PAR       X         =                                                         1.000+005        .000
 16  PAR       OH        =       MEO2                                              1.200+003   5.600+002
 17  OLE       O         =       MEO2      ACO3      X                             2.700+003   3.250+002
 18  OLE       O         =       HCHO      PAR                                     2.700+003   3.250+002
 19  OLE       OH        =       RAO2                                              3.700+004  -5.400+002
 20  OLE       O3        =       HCHO      CRIG                                    8.000-003   1.900+003
 21  OLE       O3        =       HCHO      MCRG      X                             8.000-003   1.900+003
 22  ETH       O         =       MEO2      HO2       CO                            6.000+002   8.000+002
 23  ETH       O         =       HCHO      PAR                                     6.000+002   8.000+002
 24  ETH       OH        =       RBO2                                              1.200+004  -3.820+002
 25  ETH       O3        =       HCHO      CRIG                                    2.400-003   2.560+003
 26  ACO3      NO        =       NO2       MEO2                                    1.040+004        .000
 27  RBO2      NO        =       NO2       HO2       HCHO      HCHO                1.200+004        .000
 28  RAO2      NO        =       NO2       HO2       HCHO      HCHO                1.200+004        .000
 29  MEO2      NO        =       NO2       MEO2      HCHO      X                   3.700+003        .000
 30  MEO2      NO        =       NO2       HCHO      HO2                           7.400+003        .000
 31  MEO2      NO        =                                                         9.000+002        .000
 32  RBO2      O3        =       HCHO      HCHO      HO2                           5.000+000        .000
 33  RAO2      O3        =       HCHO      HCHO      HO2                           2.000+001        .000
 34  OH        HCHO      =       CRO2      X                                       1.000+002        .000
 35  HCHO      OH        =       HO2       CO                                      9.000+003        .000
 36  HCHO      OH        =       X         ACO3                                    8.200+003        .000
 37  HCHO                =       CO                                                2.400-001        .000
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4

```
 80   HCHO               =    QQ                                   5.640-001      .000
 81   QQ                 =    HO2      HO2      CO                 8.867+003      .000
 82   QQ                 =    MEO2     MEO2     X        XCO        1.133+003      .000
 83   XCO                =    X        CO                          1.000+004      .000
 39   ACO3     NO2       =    PAN                                  7.000+003      .000
 40   PAN                =    ACO3     NO2                         2.200-002      1.350+004
 41   ACO3     HO2       =                                         1.500+004      .000
 42   MEO2     HO2       =                                         9.000+003      .000
 43   CRIG     NO        =    NO2      HCHO                        1.200+004      .000
 44   CRIG     NO2       =    NO3      HCHO                        8.000+003      .000
 45   CRIG     HCHO      =                                         2.000+003      .000
 46   MCRG     NO        =    NO2      HCHO     PAR                1.200+004      .000
 47   MCRG     NO2       =    NO3      HCHO     PAR                8.000+003      .000
 48   MCRG     HCHO      =                                         2.000+003      .000
 49   CRIG               =    CO                                   6.700+002      .000
 50   CRIG               =                                         2.400+002      .000
 51   CRIG               =    HO2      HO2      CO                 9.000+001      .000
 52   MCRG               =                                         1.500+002      .000
 53   MCRG               =    MEO2     OH       CO                 3.400+002      .000
 54   MCRG               =    MEO2     HO2                         4.250+002      .000
 55   MCRG               =    HCHO     HO2      HO2      CO        8.500+001      .000
 56   ARO      OH        =    RARO                                 6.000+003      6.000+002
 57   ARO      OH        =    HO2      OPEN                        1.450+004      4.000+002
 58   RARO     NO        =    NO2      PHEN     HO2                4.000+003      .000
 59   OPEN     NO        =    NO2      ALD2     X        APRC      6.000+003      .000
 60   APRC               =    ALD2     HCHO     CO       X         1.000+004      .000
 61   APRC               =    HCHO     HCHO     CO       CO        1.000+004      .000
 62   PHEN     NO3       =    PHO      HNO3                        5.000+003      .000
 63   PHO      NO2       =                                         4.000+003      .000
 64   PHO      HO2       =    PHEN                                 5.000+004      .000
 65   OPEN     O3        =    ALD2     X        APRC               4.000+001      .000
 66   OH       PHEN      =    HO2      APRC     PAR      HCHO      3.000+004      .000
 67   ALD2               =    HO2      ACO3     CO                 2.000-002      .000
 68   PHEN     OH        =    PHO                                  1.000+004      .000
 69   CRO2     NO        =    NO2      HCHO     ACO3     X         1.200+004      .000
 70   ALD2     OH        =    ACO3     CO                          2.500+004      .000
 71   HONO               =    OH       NO                          3.100+000      .000
 72   OH       NO        =    HONO                                 9.770+003      .000
 73   O3                 =    O1D                                  5.400-001      .000
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued)

```
 74   O1D                  =         O                                  4.440+010     .000
 75   O1D                  =         OH        OH                       6.800+009     .000
 90   OH                   =         HO2                                8.800+001     .000
 91   OH                   =         MEO2                               2.800+001     .000
 92   NR                   =         NR                                 1.000+000     .000
 99   O3                   =         O                                  1.000+000     .000
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued -3)

```
EXAMPLE 5-4

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        CITY NAME

LATITUDE     39.000

LONGITUDE     77.000

TIME ZONE    5.0

DATE         8      1   1981

TIME         800   TO   2000     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

HOUR          0       1       2       3       4       5       6       7       8

HEIGHT      250.0   410.0   620.0   810.0   950.0  1050.0  1120.0  1180.0  1220.0


INITIAL         PAR  FRACTION  .580   ETH  FRACTION  .040   OLE  FRACTION  .030

INITIAL         ARO  FRACTION  .190   HCHO FRACTION  .050   ALD2 FRACTION  .000

INITIAL         NR   FRACTION  .150

NO2/NOX       .250

THERE ARE NO ALDEHYDES IN THE MECHANISM


TRANSPORTED CONCENTRATIONS

SURFACE LAYER         OZONE     .010      HYDROCARBON   .038    NOX       .000 PPM

SURFACE LAYER         PAN       .005

ALOFT                 OZONE     .080      HYDROCARBON   .040    NOX       .000 PPM


EMISSION FRACTIONS COMPUTED FROM THE FOLLOWING

  INITIAL MIXING HEIGHT (METERS) :    250.0

  INITIAL HC CONCENTRATION (PPMC) :    1.20

  INITIAL NOX CONCENTRATION (PPM) :    .150

  HOURLY EMISSION DENSITIES (KG/KM2) :

     HOUR       1       2       3       4       5       6       7       8

     HC       50.0    50.0    50.0    25.0     5.0     5.0     5.0     5.0

     HOUR       1       2       3       4       5       6       7       8

     NOX      25.0    25.0    25.0    15.0     3.0     3.0     3.0     3.0
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued -4)

```
CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTON OF INITIAL
NON-BACKGROUND HYDROCARBON CONCENTRATION EMITTED PER HOUR)
     HOUR         1     2     3     4     5     6     7     8
     FRACTION   .280  .280  .280  .140  .028  .028  .028  .028

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF INITIAL
NON-BACKGROUND NOX CONCENTRATION EMITTED PER HOUR)
     HOUR         1     2     3     4     5     6     7     8
     FRACTION   .353  .353  .353  .212  .042  .042  .042  .042
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued -5)

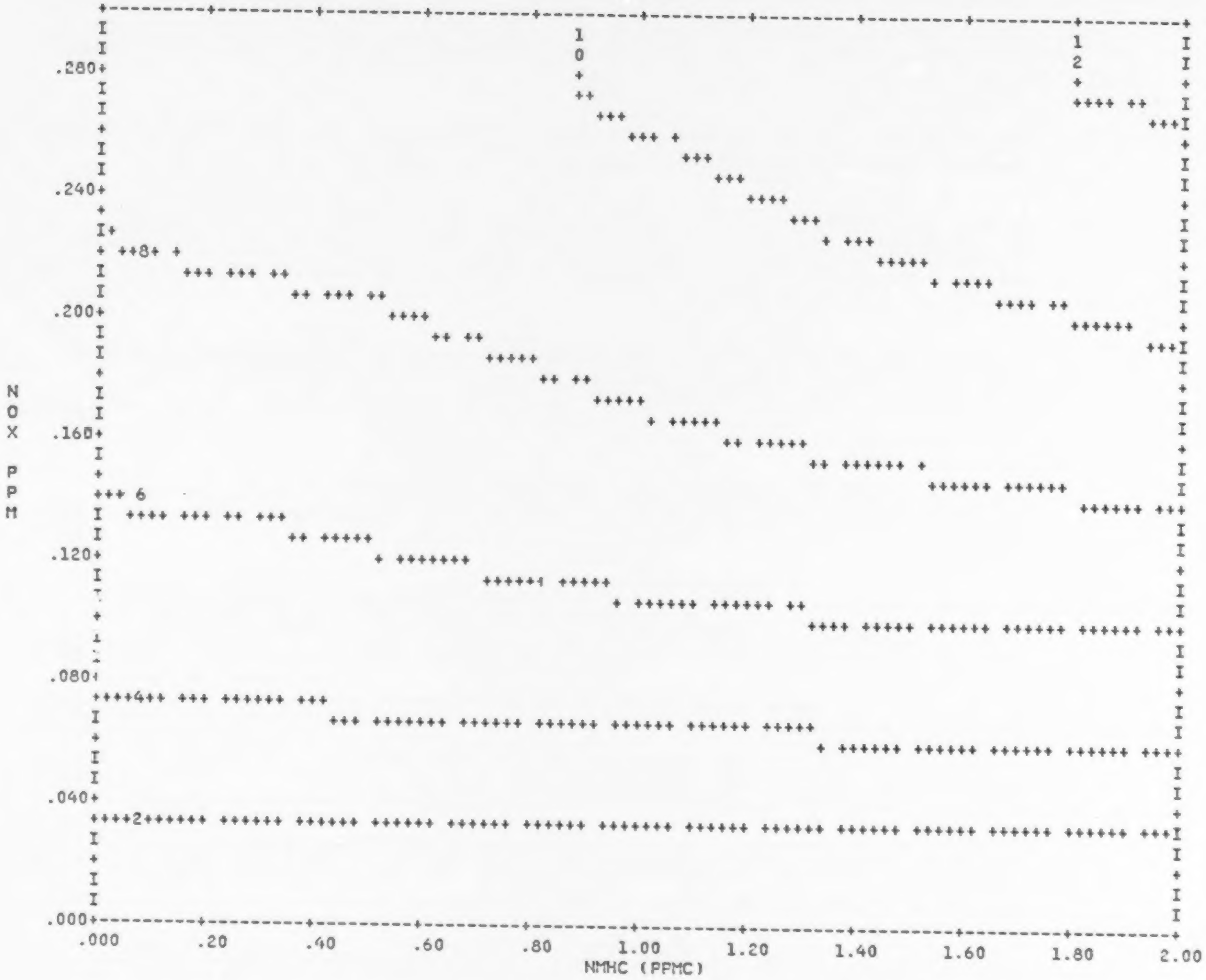
```
     HC              NOX            RATIO            NO2

   .00000          .00000          .00000          .00082
   .00000          .28000          .00000          .08861
  2.00000          .28000         7.14286          .12382
  2.00000          .00000          .00000          .00085
   .10000          .28000          .35714          .08945
  2.00000          .04360        45.87048          .02875
  1.26300          .17682         7.14286          .08529
   .70592          .09883         7.14286          .05390
   .37883          .05304         7.14286          .03191
   .21516          .03012         7.14286          .01914
  1.62000          .28000         5.78571          .11659
  1.03847          .17949         5.78571          .08270
   .57320          .09907         5.78571          .05290
   .30210          .05222         5.78571          .03116
   .17630          .03047         5.78571          .01926
  1.20000          .28000         4.28571          .10731
   .78528          .18323         4.28571          .07967
   .41807          .09755         4.28571          .05096
   .21704          .05064         4.28571          .03003
   .13225          .03086         4.28571          .01937
   .80000          .28000         2.85714          .09816
   .53526          .18734         2.85714          .07674
   .26763          .09367         2.85714          .04823
   .13856          .04850         2.85714          .02861
   .08947          .03131         2.85714          .01950
   .75899          .28000         2.71069          .09745
   .50874          .18768         2.71069          .07644
   .25437          .09384         2.71069          .04817
   .13126          .04842         2.71069          .02856
   .08491          .03132         2.71069          .01949
   .00000          .28000          .00000          .08861
   .00000          .19218          .00000          .07169 NOT MAX
   .00000          .09609          .00000          .04662
   .00000          .04839          .00000          .02788
   .00000          .03201          .00000          .01961
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued -6)

```
   2.00000          .23832          8.39203          .11299
   1.29210          .15397          8.39202          .07889
    .75177          .08958          8.39202          .05054
    .43138          .05140          8.39202          .03127
    .25292          .03014          8.39202          .01922
   2.00000          .19664         10.17072          .10103
   1.32858          .13063         10.17072          .07122
    .81974          .08060         10.17072          .04707
    .50193          .04935         10.17072          .03043
    .30631          .03012         10.17072          .01930
   2.00000          .15496         12.90618          .08633
   1.38163          .10705         12.90618          .06205
    .91308          .07075         12.90618          .04282
    .60060          .04654         12.90618          .02919
    .39106          .03030         12.90618          .01954
   2.00000          .11329         17.65443          .06820
   1.46531          .08300         17.65443          .05103
   1.05250          .05962         17.65443          .03745
    .75452          .04274         17.65443          .02737
    .53709          .03042         17.65443          .01978
   2.00000          .05771         34.65325          .03770
   1.60000          .04617         34.65324          .03026
   1.20000          .03463         34.65324          .02280
    .80000          .02309         34.65324          .01531
    .72000          .02078         34.65324          .01380
    .37950          .28000          1.35535          .09975 NOT MAX
   2.00000          .02922         68.44040          .01922
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued -7)



```
EXAMPLE 5-4

THE NO2  LINES ARE    .02000  .04000  .06000  .08000  .10000  .12000
```

FIGURE 5-4. OUTPUT FOR EXAMPLE 5-4 (continued -8)

6.0 REFERENCES

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14. J. P. Killus and G. Z. Whitten, *Technical Discussions Relating to the Use of the Carbon-Bond Mechanism in OZIPM/EKMA*, EPA-450/4-84-009, U. S. Environmental Protection Agency, Research Triangle Park, North Carolina, May 1984.

APPENDIX A

DEFAULT KINETIC MECHANISM USED IN OZIPM-2

APPENDIX A

DEFAULT KINETIC MECHANISM USED IN OZIPM-2

Number	Reaction	Rate Constant*
1.	$NO_2 + hv \longrightarrow NO + O(^3P)$	k_{vary}
2.	$O(^3P) + O_2 + M \longrightarrow O_3 + M$	$2.0 \times 10^{-5}\ ppm^{-2}min^{-1}$
3.	$O_3 + NO \longrightarrow NO_2 + O_2$	25.0
4.	$NO_2 + O_3 \longrightarrow NO_3 + O_2$	0.045
5.	$NO_2 + O(^3P) \longrightarrow NO + O_2$	1.3×10^4
6.	$NO_3 + NO \longrightarrow 2NO_2$	1.3×10^4
7.	$NO_2 + NO_3 \longrightarrow N_2O_5$	5.6×10^3
8.	$N_2O_5 \longrightarrow NO_2 + NO_3$	$22.0\ min^{-1}$
9.	$N_2O_5 + H_2O \longrightarrow 2HNO_3$	2.5×10^{-6}
10.	$NO + NO_2 + H_2O \longrightarrow 2HONO$	$1.0 \times 10^{-9}\ ppm^{-2}min^{-1}$
11.	$2HONO \longrightarrow NO + NO_2 + H_2O$	1.0×10^{-3}
12.	$HONO + hv \longrightarrow OH + NO$	k_{vary} M
13.	$OH + NO_2 \longrightarrow HNO_3$	8.0×10^3 M
14.	$OH + NO \longrightarrow HONO$	3.0×10^3
15.	$HO_2 + NO \longrightarrow NO_2 + OH$	1.2×10^3
16.	$HO_2 + HO_2 \longrightarrow HOOH + O_2$	8.4×10^3
17.	$HOOH + hv \longrightarrow 2OH$	k_{vary}
18.	$O_3 + hv \longrightarrow O(^1D)$	k_{vary}
19.	$O_3 + hv \longrightarrow O(^3P)$	k_{vary}
20.	$O(^1D) + M \longrightarrow O(^3P) + M$	8.7×10^4
21.	$O(^1D) + H_2O \longrightarrow 2OH$	5.1×10^5
22.	$OH + O_3 \longrightarrow HO_2 + O_2$	84.0
23.	$O_3 + HO_2 \longrightarrow OH + 2O_2$	2.4
24.	$PROP + OH \longrightarrow ADD$	2.5×10^4

APPENDIX A (continued)

DEFAULT KINETIC MECHANISM USED IN OZIPM-2

Number	Reaction	Rate Constant*
25.	ADD + NO ---> X + NO_2	1.0×10^3
26.	ADD + ADD ---> 2X	1.2×10^4
27.	ADD + MeO_2 ---> X + MeO	1.0×10^3
28.	ADD + C_2O_2 ---> X + C_2O	1.0×10^3
29.	ADD + C_3O_2 ---> X + C_3O	1.0×10^3
30.	X ---> HCHO + ALD2 + HO_2	1.0×10^5 min^{-1}
31.	PROP + O_3 --> OH + HO_2 + ALD2	8.0×10^{-3}
32.	PROP + O_3 ---> OH + C_2O_3 + HCHO	8.0×10^{-3}
33.	BUT + OH ---> ScO_2	1.8×10^3
34.	BUT + OH ---> C_4O_2	1.8×10^3
35.	NO + C_4O_2 ---> NO_2 + C_4O	1.8×10^3
36.	NO + ScO_2 ---> NO_2 + ScO	1.8×10^3
37.	NO + C_3O_2 ---> NO_2 + C_3O	1.8×10^3
38.	NO + C_2O_2 ---> NO_2 + C_2O	1.8×10^3
39.	NO + MeO_2 ---> NO_2 + MeO	1.8×10^3
40.	C_4O ---> HCHO + C_3O_2	7.5×10^4 min^{-1}
41.	ScO ---> ALD2 + C_2O_2	1.0×10^5 min^{-1}
42.	C_3O ---> HCHO + C_2O_2	8.0×10^3 min^{-1}
43.	C_2O ---> HCHO + MeO_2	4.0×10^3 min^{-1}
44.	C_4O + O_2 ---> ALD4 + HO_2	0.7
45.	ScO + O_2 ---> MEK + HO_2	1.4
46.	C_3O + O_2 ---> ALD3 + HO_2	0.5
47.	C_2O + O_2 ---> ALD2 + HO_2	0.4

APPENDIX A (continued)

DEFAULT KINETIC MECHANISM USED IN OZIPM-2

Number	Reaction	Rate Constant*
48.	MeO + O_2 ---> HCHO + HO_2	0.4
49.	HCHO + hv ---> stable products	k_{vary}
50.	HCHO + hv ---> $2HO_2$	k_{vary}
51.	HCHO + OH ---> HO_2	1.5×10^4
52.	ALD2 + hv ---> stable products	4.2×10^{-6} min $^{-1}$
53.	ALD2 + hv ---> MeO_2 + HO_2	k_{vary}
54.	ALD2 + OH ---> C_2O_3	1.5×10^4
55.	ALD3 + hv ---> stable proudcts	6.0×10^{-5} min^{-1}
56.	ALD3 + hv ---> C_2O_2 + HO_2	2.5×10^{-3} min^{-1}
57.	ALD3 + OH ---> C_3O_3	4.5×10^4
58.	ALD4 + hv ---> stable products	6.0×10^{-5} min^{-1}
59.	ALD4 + hv ---> C_3O_2 + HO_2	1.9×10^{-3} min^{-1}
60.	ALD4 + OH ---> C_4O_3	4.5×10^4
61.	ADD + C_4O_2 ---> X + C_4O	1.0×10^3
62.	ADD + ScO_2 ---> X + ScO	1.0×10^3
63.	C_4O_3 + NO ---> C_3O_2 + NO_2	8.0×10^2
64.	C_3O_3 + NO ---> C_2O_3 + NO_2	8.0×10^2
65.	C_2O_3 + NO ---> MeO_2 + NO_2	8.0×10^2
66.	C_4O_3 + NO_2 ---> PAN	1.0×10^2
67.	C_3O_3 + NO_2 ---> PAN	1.0×10^2
68.	C_2O_3 + NO_2 ---> PAN	1.0×10^2
69.	C_4O_2 + HO_2 ---> stable products	4.0×10^3
70.	C_3O_2 + HO_2 ---> stable products	4.0×10^3
71.	ScO_2 + HO_2 ---> stable products	4.0×10^3

APPENDIX A (continued)

DEFAULT KINETIC MECHANISM USED IN OZIPM-2

Number	Reaction	Rate Constant*
72.	$C_2O_2 + HO_2$ ---> stable products	4.0×10^3
73.	$MeO_2 + HO_2$ ---> stable products	4.0×10^3
74.	$C_4O_3 + HO_2$ ---> stable products	4.0×10^3
75.	$C_3O_3 + HO_2$ ---> stable products	4.0×10^3
76.	$C_2O_3 + HO_2$ ---> stable products	4.0×10^3

* Units of $ppm^{-1}min^{-1}$ unless otherwise indicated

Source: Dodge (1977)

Symbol	Definition
k_{vary}	diurnal 1-hour average photolytic rate constant
PROP	C_3H_6
BUT	$n\text{-}C_4H_{10}$

APPENDIX A (continued)

DEFAULT KINETIC MECHANISM USED IN OZIPM-2

Symbol	Definition
ADD	$CH_3CH(OH)CH_2OO$
X	$CH_3CH(OH)CH_2O$
MeO_2	CH_3O_2
C_2O_2	$CH_3CH_2O_2$
C_3O_2	$CH_3CH_2CH_2O_2$
C_4O_2	$CH_3CH_2CH_2CH_2O_2$
ScO_2	$CH_3CH(O_2)CH_2CH_3$
ALD2	CH_3CHO
ALD3	CH_3CH_2CHO
ALD4	$CH_3CH_2CH_2CHO$
C_2O_3	CH_3CO_3
C_3O_3	$CH_3CH_2CO_3$
C_4O_3	$CH_3CH_2CH_2CO_3$

APPENDIX B

RESTRUCTURING REACTIONS FOR OZIPM-2 FORMAT

APPENDIX B

As noted in the text of Section 3.2.1, the OZIPM-2 program requires that the mechanism conform to some rules. Specifically, no more than three reactants and four products are allowed per reaction, and stoichiometric coefficients of each product and reactant must be one. In many cases, reactions that do not conform to these restrictions can be restructured to meet the input criteria. The purpose of this appendix is to provide some suggestions on restructuring individual reactions for input to OZIPM-2.

B.1 REACTIONS WITH REACTANTS OF CONSTANT CONCENTRATION

Whenever a reaction contains a reactant whose concentration is relatively invariant with time (e.g., O_2), it can be rewritten as psuedo-lower order reaction. With this approach, the reactant with relatively constant concentration is eliminated from the reaction, but the reaction rate constant is adjusted to reflect the constant concentration. For example, consider the following reaction in which species B is assumed to be relatively constant in concentration:

$$A + B \dashrightarrow C \qquad k_1 \qquad \text{B-1}$$

where k_1 is the rate constant in $ppm^{-1}min^{-1}$. Reaction B-1 can be rewritten as follows, using the assumed constant concentration of species B (C_B)

$$A \dashrightarrow C \qquad k_{1A} \qquad \text{B-1A}$$

where

$$K_{1A} = K_1 C_B \; [=] \; min^{-1}$$

Note that the above formulation makes the mechanism more compact (requiring less computer time), and saves the user from having to introduce some way of keeping the concentration of the invariant species nearly constant throughout the simulation.

B.2 INTEGER STOICHIOMETRIC COEFFICIENTS NOT EQUAL TO ONE

Since all stoichiometric coefficients must be one in any individual reaction, some reactions may require some small adjustments. As an example, consider reaction of the form:

$$A + B \longrightarrow 2C \qquad k_2 \qquad \text{(B-2)}$$

This reaction can be easily rewritten to make it compatible with OZIPM-2 requirements:

$$A + B \longrightarrow C + C \qquad k_{2A}=k_2 \qquad \text{(B-2A)}$$

B.3 REACTIONS WITH MORE THAN FOUR PRODUCTS

A reaction that contains more than four products can be broken down into one or more reactions, each with four products or less. This is done by introducing a psuedo-species to represent a group of products in the initial reaction. The psuedo-species is then assumed to dissociate rapidly into the entities it was originally chosen to represent. To illustrate, consider the following reaction:

$$A + B \longrightarrow 2C + 2D + E \qquad k_3 \qquad \text{(B-3)}$$

First, this reaction can be rewritten as following using the approach described above:

$$A + B \longrightarrow C + C + D + D + E \qquad k_3 \qquad \text{(B-3A)}$$

Now, introducing the psuedo-species QQ to represent D + E, equation A-3A can be rewritten as follows:

$$A + B \longrightarrow C + C + D + QQ \qquad k_3 \qquad \text{(B-3B)}$$

$$QQ \longrightarrow D + E \qquad k_{fast} \qquad \text{(B-3C)}$$

To insure that no appreciable buildup occurs in the concentration of QQ, the value of k_{fast} in equation B-3C should be relatively fast compared to k_3 (say on the order of 1×10^{10} min^{-1}).

B.4 REACTIONS WITH NON-INTEGER STOICHIOMETRIC COEFFICIENTS

In some chemical mechanisms, one or more reactions may have stoichiometric coefficients that are not only different from one, but also non-integer as well. In such cases, the single reaction must be broken down into two or more reactions that are equivalent in a kinetic sense. Although such situations could be treated on a case-by-case basis, some generalizations can be made. Consider, for example, the general reaction shown below:

$$A + B \dashrightarrow cC + dD + eE + fF \qquad k_4 \qquad (B\text{-}4)$$

In this equation, the upper case letters refer to the species names, the lower case letters represent the stoichiometric coefficients, and the products are ordered such that $0 \leq c \leq d \leq e \leq f \leq 1.0$. Then, equation (B-4) can be rewritten as follows:

$$A + B \dashrightarrow C + D + E + F \qquad k_{4A} \qquad (B\text{-}4A)$$

$$A + B \dashrightarrow D + E + F \qquad k_{4B} \qquad (B\text{-}4B)$$

$$A + B \dashrightarrow E + F \qquad k_{4C} \qquad (B\text{-}4C)$$

$$A + B \dashrightarrow F \qquad k_{4D} \qquad (B\text{-}4D)$$

$$A + B \dashrightarrow \qquad k_{4E} \qquad (B\text{-}4E)$$

where

$$k_{4A} = ck_4 \qquad (B\text{-}4F)$$

$$k_{4B} = (d-c)\ k_4 \qquad (B\text{-}4G)$$

$$k_{4C} = (e-d)\ k_4 \qquad (B\text{-}4H)$$

$$k_{4D} = (f-d)\ k_4 \qquad (B\text{-}4I)$$

$$k_{4E} = (1.0-f)k_4 \qquad (B\text{-}4J)$$

Thus, in general, the equation B-4 would be replaced in the mechanism by the set of reactions (B-4A) through (B-4E). Of course, should any of the rate constants turn out to be zero, according to the equations (B-4F) through (B-4J), then that particular reaction could be eliminated from the mechanism.

To illustrate the generalized procedure just discussed, consider the following reaction:

$$OLE + O_3 \dashrightarrow 0.07\ RO + 0.61\ RO2 + HCHO \quad k_5 = 0.00513\ ppm^{-1}min^{-1} \quad (B\text{-}5)$$

Using the procedure discussed above, let c=0.0, d=0.07, e=0.61, and f=1.0. Then, using the generalized expressions in equations B-4A through B-4J, reaction B-5 above can be rewritten as follows

$$OLE + O_3 = RO + RO2 + HCHO \quad k_{5A} = 0.000359\ ppm^{-1}min^{-1} \quad (B\text{-}5A)$$

$$OLE + O_3 = RO2 + HCHO \quad k_{5B} = 0.00277\ ppm^{-1}min^{-1} \quad (B\text{-}5B)$$

$$OLE + O_3 = HCHO \quad k_{5C} = 0.00200\ ppm^{-1}min^{-1} \quad (B\text{-}5C)$$

These three equations would then be used in the OZIPM-2 inputs to represent the single reaction B-5.

APPENDIX C

PROGRAM SOURCE LISTING

```
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KPH(9)
      COMMON /EMIS/ NEM,EM(16),EMHC(16),EMNOX(16),ESRT(2),ESTOP,ESLP,EHS
     1LP,ENSLP,EC(80),ECHC(80),ECXN(80)
      COMMON /MIX/ MMIX,BMIX(16),STRM,STOPM,DC(45),TSTART
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /TITL/ ITTL(18)
      COMMON /NEED/ HC,XN,NL,NRTO,PTS(20),OZP(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICZ,DIGZ,CHRZ
      COMMON /VVLBL/ FCTR,DIST,CHRSIZ,NNCHR,OZBL
      COMMON /ALOFT/FALALD(4)
      COMMON /SURFAC/FINALD(4)
      COMMON /SUNLIT/ XJ(47,10),SIGMO(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(16),XZ(16),K(16),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL,MA
     3XJ
      COMMON /WRTREP/PLACE(6),EMMHC(16),EMMNX(16),MEMFLG,HCB,XNXB,HINIT
      COMMON /MIXING/ DSTRT,DEND,AMC(5),BMC(5),CMC(5),FD(6),FG(6),
     1AMIX(16),DL,TTMAX,SRISE,SRMIN,DELH,TDIL,NMIX
      COMMON/EKMART/BCO3,BCRAT,DELNOX,ICHTRN,IRANGE,FOZIN,FOZAL,FHCIN,
     1FHCAL,FXNIN,FXNAL
      DIMENSION F(21), X(7)
      DIMENSION  XRTC(76),CHRD(8)
      INTEGER SPECIS,HCSPEC,ALDSPC,PLSP,CHRD
      DATA ISPD/4HISOP/,ICAL/4HCALC/,IACR/4HACCU/,IDIL/4HDILU/,IPLC/4HPL
     1AC/,IEMS/4HEMIS/,IRDY/4HALRE/,IBLK/4H    /,IPLT/4HPLOT/,ITRN/4HTRA
     2N/,ITIT/4HTITL/,IRCT/4HREAC/,ITIM/4HTIME/,IMCH/4HMECH
     3/,INIT/4HINIT/,IMIX/4HMIXI/,ISPC/4HSPEC/,
     4IEKMA/4HEKMA/,IMASS/4HMASS/
      DATA CHRD/'O3  ',' OZO','    ',' ISO','H   ',
     *'PLET','NO2 ','NO  '/
      DATA NC/11/,KALCMP/0/,KS1/0/,JS/0/
      WRITE(IOUT,117)
      CALL PHOT
      CALL CCMIX
C
C OPTIONS LOOP
C
    5 READ(IN,290) IOPT,(X(I),I=1,6)
      IF (IOPT.NE.ISPD) GO TO 20
      IF (ABS(X(1)).NE.0.) HC=X(1)
      IF (ABS(X(2)).NE.0.) XN=X(2)
      IF (ABS(X(4)).NE.0.) INFO=-1
      IF (ABS(X(3)).NE.0.) NL=IFIX(X(3)+0.1)
      IF (ABS(X(3)).NE.0.) READ(IN,300) (OZP(I),I=1,NL)
      IF (ABS(X(5)).NE.0.) FCTR=X(5)
      CALL REPRT
      CALL RLINE (NC,F,KS1,JS)
      CALL LINER (SIG,KALCMP,F)
      INFO=0
      GO TO 5
   20 IF (IOPT.NE.ICAL) GO TO 35
      NPTO=1
      IF (ABS(X(3)).NE.0.) INFO=1
      CALL REPRT
      TPRNT=60.
      TSTEP=60.
      IF (ABS(X(4)).NE.0.) TPRNT=X(4)
      IF (ABS(X(5)).NE.0.) TSTEP=X(5)
      CALL SIM (X(1),X(2),ZN,1)
      IF (TM.GT.0.) WRITE (IOUT,310) PLSP,ZN,TM
      IF (TM.LE.0.) WRITE (IOUT,335) PLSP,ZN
      CALL LINPRT (X(1),X(2))
      NPTO=0
      INFO=0
      GO TO 5
   35 IF (IOPT.NE.IACR) GO TO 40
      IF (ABS(X(1)).NE.0.) NC=IFIX(X(1)+0.1)
      IF ((NC/2).EQ.((NC+1)/2)) NC=NC+1
      IF (ABS(X(2)).NE.0.) MR=IFIX(X(2)+0.1)
      IF (ABS(X(3)).NE.0.) ERR=X(3)
      IF (ABS(X(4)).NE.0.) SIG=X(4)
      IF (ABS(X(5)).NE.0.) SIGMA=X(5)
      IF (ABS(X(6)).NE.0.) NGO=0
      GO TO 5
   40 IF (IOPT.NE.IPLC) GO TO 45
      IF (ABS(X(1)).NE.0.) SLA=X(1)
      IF (ABS(X(2)).NE.0.) SLO=X(2)
      IF (ABS(X(3)).NE.0.) TZ=X(3)
      IF (ABS(X(4)).NE.0.) IY=IFIX(X(4)+0.01)
      IF (ABS(X(5)).NE.0.) IM=IFIX(X(5)+0.01)
      IF (ABS(X(6)).NE.0.) ID=IFIX(X(6)+0.01)
      IF (ABS(X(1)).NE.0..OR.ABS(X(2)).NE.0.)
     *READ(IN,330) (PLACE(I),I=1,6)
      CALL FHOT
      CALL CCMIX
      GO TO 5
   45 IF (IOPT.NE.IDIL) GO TO 50
      IF (ABS(X(1)).NE.0.) Z1=X(1)
      IF (ABS(X(2)).NE.0.) Z2=X(2)
      IF (ABS(X(3)).NE.0.) DSTRT=X(3)
      IF (ABS(X(4)).NE.0.) DEND=X(4)
      CALL CCMIX
      BMIX(1)=-3.
      GO TO 5
   50 IF (IOPT.NE.IMIX) GO TO 60
      MMIX=IFIX(X(1)+0.1)+1
      DO 55 I=1,5
   55 BMIX(I)=X(I+1)
      IF (MMIX-5.GT.0) READ(IN,300) (BMIX(I),I=6,MMIX)
      CALL MIXSET
      Z1=BMIX(1)
      Z2=BMIX(MMIX)
      TSRT=0.
      DTIM=STOPM
      GO TO 5
   60 IF (IOPT.NE.IEMS) GO TO 85
      MEMFLG=0
      IF(X(1).LT.0.) NEM=IFIX(X(1)-0.1)
      IF(X(1).GT.0.) NEM=IFIX(X(1)+0.1)
      IEM=IFIX(ABS(X(1))+0.1)
      ESTOP=IEM*60.
      IF (X(1).LT.-0.99999999) GO TO 70
      DO 65 I=1,5
   65 EM(I)=ABS(X(I+1))
      IF (NEM-5.GT.0) READ(IN,300) (EM(I),I=6,NEM)
      CALL EMISS(NEM,EM,EC)
      EMHC(1)=-3.
      EMNOX(1)=-3.
      GO TO 5
   70 DO 75 I=1,5
   75 EMHC(I)=X(I+1)
      IF (EMHC(1).LT.-0.0001) GO TO 80
      IF (IEM-5.GT.0) READ(IN,300) (EMHC(I),I=6,IEM)
      CALL EMISS (IEM,EMHC,ECHC)
   80 READ(IN,300) (EMNOX(I),I=1,7)
      IF (EMNOX(1).LT.-0.0001) GO TO 5
      IF (IEM-7.GT.0) READ(IN,300) (EMNOX(I),I=8,IEM)
      CALL EMISS (IEM,EMNOX,ECXN)
      GO TO 5
   85 IF (IOPT.NE.IPLT) GO TO 135
```

```
      KALCMP=1
      FCTR=0.6
      HC1=8.5
      XN1=5.95
      CHRZ=0.10
      IF (ABS(X(1)).NE.0.) FCTR=X(1)
      PLTGRD=X(2)
      IF (ABS(X(3)).NE.0.) HC1=X(3)
      IF (ABS(X(4)).NE.0.) XN1=X(4)
      IF (ABS(X(5)).NE.0.) CHRZ=X(5)
      IF (ABS(X(6)).NE.0.) CHRSIZ=X(6)
      DIGZ=CHRZ
      TICZ=CHRSIZ
      GO TO 5
  135 IF (IOPT.NE.IRCT) GO TO 140
      KHC=IFIX(X(1)+0.1)
      IF (ABS(X(2)).NE.0.) XNF(1)=X(2)
      IF (ABS(X(2)).NE.0.) XNF(2)=1.-X(2)
      KAD=IFIX(X(3)+0.1)
      IF (KHC.GT.0) READ(IN,300) (RCTY(I),I=1,KHC)
      IF (KAD.GT.0) READ(IN,300) (ALDX(I),I=1,KAD)
      GO TO 5
  140 IF (IOPT.NE.ISPC) GO TO 160
      READ(IN,290) PLSP
      DO 145 I=1,NS
      IF (SPECIS(I).NE.PLSP) GO TO 145
      KOZ=I
      GO TO 150
  145 CONTINUE
      WRITE (IOUT,440) PLSP
      STOP
  150 IF (PLSP.EQ.CHRD(1)) GO TO 5
      IF (ITTL(3).NE.CHRD(2)) GO TO 5
      DO 155 I=1,18
  155 ITTL(I)=CHRD(3)
      ITTL(1)=PLSP
      ITTL(2)=CHRD(4)
      ITTL(4)=CHRD(5)
      ITTL(3)=CHRD(6)
      GO TO 5
  160 IF (IOPT.NE.ITIT) GO TO 165
      READ(IN,295) (ITTL(I),I=1,18)
      GO TO 5
  165 IF (IOPT.NE.ITRN) GO TO 175
      OZIN=X(1)
      OZAL=X(2)
      HCIN=X(3)
      HCAL=X(4)
      XNIN=X(5)
      XNAL=X(6)
      IF (HCIN.GT.-0.0000001) GO TO 170
      JIN=IFIX(ABS(HCIN)+0.1)
      READ(IN,300) HCIN,(FINHC(I),I=1,JIN)
      IF (NALD.GT.0) READ(IN,300) (FINALD(I),I=1,4)
  170 IF (HCAL.GT.-0.0000001) GO TO 5
      JAL=IFIX(ABS(HCAL)+0.1)
      READ(IN,300) HCAL,(FALHC(I),I=1,JAL)
      IF (NALD.GT.0) READ(IN,300) (FALALD(I),I=1,4)
      GO TO 5
  175 IF (IOPT.NE.INIT) GO TO 180
      NI=IFIX(ABS(X(1))+0.1)
      READ(IN,385) (REACT(I),I=1,NI)
      READ(IN,300) (C(I),I=1,NI)
      GO TO 5
  180 IF (IOPT.NE.IRDY) GO TO 220
      KS1=IFIX(X(1)+0.1)
      KK=0
      JS=1
      IF (KK.EQ.KS1) GO TO 5
      WRITE (IOUT,320) PLSP
      DO 185 I=1,4
      READ(IN,300) HCC,XNN,OC(I)
      IF (XNN.NE.0.0) RTO1=HCC/XNN
      IF (XNN.EQ.0.0) RTO1=0.00000
      WRITE (IOUT,325) HCC,XNN,RTO1,OC(I)
      KK=KK+1
      IF (I.EQ.2) HCLL(MR)=XNN
      IF (I.NE.3) GO TO 185
      RTO(1)=RTO1
      F(1)=SQRT(RTO1*RTO1+1.)
      RHO(MR,1)=F(1)*XNN
      OZN(MR,1)=OC(3)
      HCE=0.98*HCC
      NCE=1
      IF (KK.EQ.KS1) GO TO 5
  185 CONTINUE
      IF (NC.EQ.1) GO TO 200
  190 DO 195 I=1,2
      HCS=HCC
      READ(IN,300) HCC,XNS,OS(I)
      RTO2=HCC/XNS
      WRITE (IOUT,325) HCC,XNS,RTO2,OS(I)
      KK=KK+1
      IF (KK.EQ.5) HCG=HCC
      IF (KK.EQ.5) OHC=OS(I)
      IF (KK.EQ.6) XNG=XNS
      IF (KK.EQ.6) OXN=OS(I)
      IF (KK.EQ.KS1) GO TO 5
  195 CONTINUE
  200 JK=MR-1
      NCR=(NC+1)/2
      DO 215 I=1,NC
      IF (JK+I.EQ.1) GO TO 215
  205 READ(IN,300) HCC,XNN,ZN
      IF (HCC.GT.HCE) NCE=NCE+1
      IF (JK.EQ.MR.AND.XNN.GT.0.) RTO(I)=HCC/XNN
      IF (JK.EQ.MR.AND.XNN.LE.0.) RTO(I)=HCC*1.0E7
      IF (JK.EQ.MR) F(I)=SQRT(RTO(I)*RTO(I)+1.)
      WRITE (IOUT,325) HCC,XNN,RTO(I),ZN
      IF (JK.LT.MR) GO TO 210
      IF (RTO(I).GT.1.02*RTO2.OR.RTO(I).LT.0.98*RTO2) GO TO 210
      RHO(MR,I)=SQRT(HCE*HCE*1.041232+XNS*XNS)
      OZN(MR,I)=OS(2)
      JK=MR-1
      NCE=NCE+1
      JS=JS+1
  210 OZN(JK,I)=ZN
      RHO(JK,I)=SQRT(HCC*HCC+XNN*XNN)
      IF (HCC.LE.0.AND.I.EQ.NCR) HCLL(JK)=XNN
      IF (XNN.LE.1.0E-7.AND.I.EQ.NC) XNLL(JK)=HCC
      KK=KK+1
      IF (KK.EQ.KS1) GO TO 5
      JK=JK-1
      IF (JK.GT.0) GO TO 205
      IF (NCE.EQ.(NC+1)/2) GO TO 190
  215 JK=MR
      GO TO 190
  220 IF (IOPT.NE.IMCH) GO TO 280
      NX=IFIX(ABS(X(1))+0.1)
      IP=IFIX(ABS(X(2))+0.1)
      NHC=IFIX(ABS(X(3))+0.1)
      NALD=IFIX(ABS(X(4))+0.1)
      KFACT=IFIX(ABS(X(6))+0.1)
      IF (ABS(X(5)).NE.0.) TEMP=X(5)
      IF (IP.NE.0) READ(IN,300) (XRTC(I),I=1,IP)
      IF (IP.EQ.0) GO TO 230
      DO 225 I=1,IP
  225 IPH(I)=IFIX(XRTC(I)+0.1)
  230 IF(KFACT.NE.0) READ(IN,300) (XRTC(I),I=1,KFACT)
      IF(KFACT.EQ.0) GO TO 232
      DO 231 I=1,KFACT
  231 KPH(I)=IFIX(XRTC(I)+0.1)
  232 CONTINUE
      IF (NHC.NE.0) READ(IN,385) (HCSPEC(I),I=1,NHC)
      IF (NHC.NE.0) READ(IN,300) (CARB(I),I=1,NHC)
      IF (NALD.NE.0) READ(IN,385) (ALDSPC(I),I=1,NALD)
      IF (NALD.NE.0) READ(IN,300) (ALDCRB(I),I=1,NALD)
      CALL MCHSET (NX,1)
      DO 250 J=1,NS
      DO 235 I=1,NHC
      IF (SPECIS(J).NE.HCSPEC(I)) GO TO 235
      IH(I)=J
      GO TO 250
  235 CONTINUE
      IF (NALD.EQ.0) GO TO 245
      DO 240 I=1,NALD
      IF (SPECIS(J).NE.ALDSPC(I)) GO TO 240
      IALD(I)=J
      GO TO 250
  240 CONTINUE
  245 IF (SPECIS(J).EQ.CHRD(7) ) INOX(1)=J
      IF (SPECIS(J).EQ.CHRD(8)) INOX(2)=J
      IF (SPECIS(J).EQ.PLSP) KOZ=J
  250 CONTINUE
      NSPARS=1
      GO TO 5
  280 IF (IOPT.NE.ITIM) GO TO 285
      START=0.
      STOPP=600.
      JSTRT=800
      JSTOP=1900
      IF (ABS(X(2)).EQ.0.) GO TO 5
      JSTRT=IFIX(X(1)+0.1)
      JSTOP=IFIX(X(2)+0.1)+100
      JMIN=JSTRT-((JSTRT/100)*100)
      TMIN1=FLOAT((JSTRT/100)*60+JMIN)
      JMIN=JSTOP-((JSTOP/100)*100)
      TMIN2=FLOAT((JSTOP/100)*60+JMIN)
      STOPP=TMIN2-TMIN1
      STOPP=STOPP-60.
      TSTART=TMIN1
      CALL PHOT
      GO TO 5
  285 IF (IOPT.NE.IEKMA) GO TO 500
      BCO3=X(1)
      BCPAT=X(2)
      DELNOX=X(3)
      ICHTRN=IFIX(X(4)+0.1)
      IRANGE=IFIX(X(5)+0.1)
      FOZIN=OZIN
      FOZAL=OZAL
      FHCIN=HCIN
      FHCAL=HCAL
      FXNIN=XNIN
      FXNAL=XNAL
      IF(ICHTRN.EQ.0) GO TO 286
      READ(IN,300) (XRTC(J),J=1,6)
      IF(XRTC(1).GT.0.) FOZIN=XRTC(1)
      IF(XRTC(2).GT.0.) FOZAL=XRTC(2)
      IF(XRTC(3).GT.0.) FHCIN=XRTC(3)
      IF(XRTC(4).GT.0.) FHCAL=XRTC(4)
      IF(XRTC(5).GT.0.) FXNIN=XRTC(5)
      IF(XRTC(6).GT.0.) FXNAL=XRTC(6)
  286 CONTINUE
      CALL REFRT
      CALL EKMA
      GO TO 5
  500 IF(IOPT.NE.IMASS) GO TO 700
      IEM=IFIX(ABS(X(1))+0.1)
      NEM=-IEM
      HCB=X(2)
      XNXB=X(3)
      HINIT=X(4)
      ESTOP=IEM*60.
      READ(IN,300) (EMMHC(I),I=1,7)
      IF(IEM.GT.7) READ(IN,300) (EMMHC(I),I=8,IEM)
      READ(IN,300) (EMMNX(I),I=1,7)
      IF(IEM.GT.7) READ(IN,300) (EMMNX(I),I=8,IEM)
      IF(HCB.LE.0.0.OR.XNXB.LE.0.0) GO TO 630
      IF(HINIT.LE.0.0) GO TO 630
      DO 600 I=1,IEM
      EMHC(I)=EMMHC(I)/(HCB*HINIT*0.595)
      EMNOX(I)=EMMNX(I)/(XNXB*HINIT*1.890)
  600 CONTINUE
      CALL EMISS(IEM,EMHC,ECHC)
      CALL EMISS(IEM,EMNOX,ECXN)
      MEMFLG=1
      GO TO 5
  630 WRITE(IOUT,450)
      STOP
  700 IF (IOPT.NE.IBLK) WRITE (IOUT,305) IOPT
      IF (IOPT.NE.IBLK) GO TO 5
      WRITE(IOUT,720)
      STOP
C
C
C
  117 FORMAT(1H1,//////////1X,T39,54('*')/1X,T39,'*',T92,'*'/
     +1X,T39,'*',2X,'OZONE ISOPLETH PLOTTING WITH OPTIONAL MECHANISMS'
     +,2X,'*'/1X,T39,'*',T92,'*'/1X,T39,'*',T62,'O Z I P M',T92,'*'/1X,
     +T39,'*',T92,'*'/1X,T39,'*',T62,'VERSION 2',T92,'*'/1X,
     +T39,'*',T92,'*'/1X,T39,'*',T60,'AUGUST, 1984',T92,'*'/1X,
     +T39,'*',T92,'*'/1X,T39,54('*'))
  290 FORMAT (A4,6X,7F10.2)
  295 FORMAT (18A4)
  300 FORMAT (7F10.5)
  305 FORMAT (1H1,24HTHE OPTIONS INSTRUCTION ,A4,21H CANNOT BE PROCESSED
     1.)
  310 FORMAT (1H0,30X,21HMAXIMUM ONE HOUR AVE ,A4,1X,3H = ,F7.5,12H CENT
     1ERED AT,F5.0,9H MINUTES.)
  320 FORMAT (1H1,//,14X,36HTHE FOLLOWING RESULTS WERE READ IN. ////1H ,
     116X,2HHC,18X,3HNOX,15X,5HRATIO,17X,A4)
  325 FORMAT (1H0,4F20.5)
  330 FORMAT (6A4,6X,2A1)
  335 FORMAT (1H0,30X,8HMAXIMUM ,A4,1X,43H NOT REACHED, THE LAST ONE HOU
     1R AVERAGE WAS,F7.5,5H PPM.)
  385 FORMAT (7(A4,6X))
  440 FORMAT (1H1,39X,8HSPECIES ,A4,38H IS NOT FOUND IN THE KINETIC MECH
     1ANISM)
  450 FORMAT(1H1,'ERROR IN INPUT DATA FOR OPTION MASSEMIS')
  720 FORMAT(1H1)
      END
```

SUBROUTINE PHOT

```
      SUBROUTINE PHOT
C
C     ****    RATE CONSTANT CALCULATIONS FOR FIRST ORDER PHOTOCHEMICAL RE
C
      REAL K
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(016),XZ(016),K(016),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL
     3,MAXJ
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KPH(9)
      DIMENSION D(2), C(27), W(45), V(5), TMS(16), CC(45)
      DATA D/0.0,0.0/
C
      IEND=16
      NTM=IEND
      TIME=JSTRT
      DO 5 II=1,IEND
C
C     ****    CALL SUBROUTINE TO COMPUTE ZENITH ANGLES FROM TIME OF DAY
C
      XC=0.0
      TSTD=TIME-100.
      IF (TSTD.LT.0.) TSTD=TSTD+2400.
      CALL SOLAR (SLA,SLO,TZ,IY,IM,ID,TSTD,XC,5)
      ITIME(II)=TIME
      XZ(II)=90.-XC
      TIME=CLOCK(TIME,IINC)
    5 CONTINUE
C
      DO 20 L=1,MAXL
      SPECIE=SPEC(L)
      ISTRT=(MNLM(L)-LAM1)/INC+1
      ISTOP=(MXLM(L)-LAM1)/INC+1
      DO 10 M=1,MAXZ
C
C     ****    CALL SUBROUTINE TO CALCULATE RATE CONSTANTS
C
      CALL RATE (L,M,MNLM(L),MXLM(L),RTCON(M))
   10 CONTINUE
C
C     ****    CALL FIRST SUBROUTINE FOR SPLINE INTERPOLATION OF RATE CONS
C
      CALL SPLNA (MAXZ,Z,RTCON,2,D,C,W)
      DO 15 II=1,IEND
      V(1)=XZ(II)
      P(II,L)=0.
      K(II)=P(II,L)
      IF (V(1).GT.90.0) GO TO 15
C
C     ****    CALL SECOND SUBROUTINE IN SPLINE INTERPOLATION SCHEME
C
      CALL SPLNB (MAXZ,Z,RTCON,C,V)
      P(II,L)=AMAX1(0.0,V(2))
      K(II)=P(II,L)
   15 CONTINUE
C
   20 CONTINUE
C     DETERMINE TIME OF SOLAR NOON
      DO 25 I=2,IEND
      IF (XZ(I).GT.XZ(I-1)) GO TO 30
   25 CONTINUE
      I=IEND
   30 TIME=ITIME(I-1)
      XA=XZ(I-1)
      DO 35 I=1,60
      SPECIE=TIME
      TIME=CLOCK(TIME,1)
      TSTD=TIME-100.
      IF (TSTD.LT.0.) TSTD=TSTD+2400.
      XB=XA
      CALL SOLAR (SLA,SLO,TZ,IY,IM,ID,TSTD,XC,5)
      XA=90.-XC
      IF (XA.GT.XB) GO TO 40
   35 CONTINUE
   40 DO 45 I=1,IEND
      TMS(I)=60.*FLOAT(I-1)
   45 P(I,3)=P(I,3)+P(I,MAXL)
      DO 200 L=1,8
      KST=0
      KEND=0
      DO 50 J=1,IEND
      IF(P(J,L).LE.0.) GO TO 50
      KST=J
      GO TO 51
   50 CONTINUE
   51 DO 60 J=1,IEND
      NMM=IEND+1-J
      IF(P(NMM,L).LE.0.0) GO TO 60
      KEND=NMM
      GO TO 61
   60 CONTINUE
   61 CONTINUE
      IF(KST.GT.1) KST=KST-1
      IF(KEND.LT.IEND) KEND=KEND+1
      NMM=KEND-KST+1
      CALL SPLNA (NMM,TMS(KST),P(KST,L),2,D,CC,W)
      KEND=KEND-1
      JJ=0
      JEND=IEND-1
      DO 100 J=1,JEND
      IF(J.LT.KST) GO TO 80
      IF(J.GT.KEND) GO TO 80
      JJ=JJ+1
      CF(3*J-2,L)=CC(3*JJ-2)
      CF(3*J-1,L)=CC(3*JJ-1)
      CF(3*J,L)=CC(3*JJ)
      GO TO 100
   80 CF(3*J-2,L)=0.0
      CF(3*J-1,L)=0.0
      CF(3*J,L)=0.0
  100 CONTINUE
  200 CONTINUE
      RETURN
      END
```

SUBROUTINE RATE

```
      SUBROUTINE RATE (L,NZ,MINLAM,MAXLAM,SUM)
      REAL K
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(016),XZ(016),K(016),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL
     3,MAXJ
C
C    ****    THIS SUBROUTINE CALCULATES A SINGLE RATE CONSTANT ACCORDING
C    ****        THE GIVEN INPUTS
C
      SUM=0.0
      DO 5 I=MINLAM,MAXLAM,INC
      II=(I-LAM1)/INC+1
      IJ=II
      IF (L.EQ.MAXL) IJ=II-16
      SUM=SUM+XJ(II,NZ)*1.0E+15*SIGMA(IJ,L)*PHI(IJ,L)
    5 CONTINUE
      SUM=SUM*60.
      RETURN
      END
```

SUBROUTINE SOLAR

```
      SUBROUTINE SOLAR (SLA,SLO,TZ,IY,IM,ID,TIME,D,NV)
C***
C***     SLA...  LATITUDE (DEG)  SOUTH = MINUS
C***     SLO...  LONGITUDE (DEG)  EAST = MINUS
C***     TZ...  TIME ZONE
C***            ALSO INCLUDES FRACTION IF LOCAL TIME IS NOT
C***             STANDARD MERIDIAN TIME.  E.G. POONA, INDIA 5.5
C***     IY..  YEAR
C***     IM..  MONTH
C***     ID..  DAY
C***     TIME.. LOCAL STANDARD TIME IN HOURS AND MINUTES.
C***            1 30 PM = 1330  ** STANDARD TIME **
C***     D..  RETURNED VALUE
C***     NV..  VALUE TO BE RETURNED, SELECTED AS FOLLOWS....
C***           1...  DECLINATION (DEG.)
C***           2...  EQUATION OF TIME ADJUSTMENT (HRS.)
C***           3...  TRUE SOLAR TIME (HRS.)
C***           4...  HOUR ANGLE (DEG.)
C***           5...  SOLAR ELEVATION (DEG.)
C***           6...  OPTICAL AIRMASS
C***     0 ( NV ( 7.  OTHERWISE, D = 9999.
C***
      DIMENSION MD(11)
      DATA MD/31,29,31,30,31,30,2*31,30,31,30/
      DATA A,B,C,SIGA/0.15,3.885,1.253,279.9348/
      RAD=572957.75913E-4
      SDEC=39784.988432E-5
      RE=1.
      IF (SLO.LT.0.) RE=-1.
      KZ=TZ
      TC=(TZ-KZ)*RE
      TZZ=KZ*RE
      SLB=SLA/RAD
      K=ID
      TIMH=TIME/100.
      I=TIMH
      TIMLOC=(TIMH-I)/0.6+I+TC
      IMC=IM-1
      IF (IMC.LT.1) GO TO 10
      DO 5 I=1,IMC
    5 K=K+MD(I)
   10 LEAP=1
      NL=MOD(IY,4)
      IF (NL.LT.1) LEAP=2
      SMER=TZZ*15.
      TK=((SMER-SLO)*4.)/60.
      KR=1
      IF (K.GE.61.AND.LEAP.LT.2) KR=2
      DAD=(TIMLOC+TZZ)/24.
      DAD=DAD+K-KR
      DF=DAD*360./365.242
      DE=DF/RAD
      DESIN=SIN(DE)
      DECOS=COS(DE)
      DESIN2=SIN(DE*2.)
      DECOS2=COS(DE*2.)
      SIG=SIGA+DF+1.914827*DESIN-0.079525*DECOS+0.019938*DESIN2-0.00162*
     1DECOS2
      SIG=SIG/RAD
      DECSIN=SDEC*SIN(SIG)
      EFFDEC=ASIN(DECSIN)
      IF (NV.NE.1) GO TO 15
      D=EFFDEC*RAD
      RETURN
   15 EQT=0.12357*DESIN-0.004289*DECOS+0.153809*DESIN2+0.060783*DECOS2
      IF (NV.NE.2) GO TO 20
      D=EQT
      RETURN
   20 TST=TK+TIMLOC-EQT
      IF (NV.NE.3) GO TO 25
      D=TST
      IF (D.LT.0.) D=D+24.
      IF (D.GE.24.) D=D-24.
      RETURN
   25 HRANGL=ABS(TST-12.)*15.
      IF (NV.NE.4) GO TO 30
      D=HRANGL
      RETURN
   30 HRANGL=HRANGL/RAD
      SOLSIN=DECSIN*SIN(SLB)+COS(EFFDEC)*COS(SLB)*COS(HRANGL)
      SOLEL=ASIN(SOLSIN)*RAD
      IF (NV.NE.5) GO TO 35
      D=SOLEL
      RETURN
   35 IF (NV.NE.6) GO TO 40
      IF (SOLEL.LE.0.) GO TO 40
      TK=SOLEL+B
      E=1./TK**C
      D=1./(A*E+SOLSIN)
      RETURN
   40 D=9999.
      RETURN
      END
```

SUBROUTINE SPLNA

```
      SUBROUTINE SPLNA (N,X,Y,J,D,C,W)
      DIMENSION X(10), Y(10), D(2), C(30), W(30)
C     ------------------------------------------------------------------
C             OVER THE INTERVAL X(I) TO X(I+1), THE INTERPOLATING
C             POLYNOMIAL
C                  Y=Y(I)+A(I)*Z+B(I)*Z**2+E(I)*Z**3
C             WHERE Z=(X-X(I))/(X(I+1)-X(I))
C             IS USED. THE COEFFICIENTS A(I),B(I) AND E(I) ARE COMPUTED
C             BY SPLNA AND STORED IN LOCATIONS C(3*I-2),C(3*I-1) AND
C             C(3*I) RESPECTIVELY.
C             WHILE WORKING IN THE ITH INTERVAL,THE VARIABLE Q WILL
C             REPRESENT Q=X(I+1) - X(I), AND Y(I) WILL REPRESENT
C             Y(I+1)-Y(I)
C     ------------------------------------------------------------------
      Q=X(2)-X(1)
      YI=Y(2)-Y(1)
      IF (J.EQ.2) GO TO 5
C     ------------------------------------------------------------------
C             IF THE FIRST DERIVATIVE AT THE END POINTS IS GIVEN,
C             A(1) IS KNOWN, AND THE SECOND EQUATION BECOMES
C             MERELY B(1)+E(1)=YI - Q*D(1).
C     ------------------------------------------------------------------
      C(1)=Q*D(1)
      C(2)=1.0
      W(2)=YI-C(1)
      GO TO 10
C     ------------------------------------------------------------------
C             IF THE SECOND DERIVATIVE AT THE END POINTS IS GIVEN
C             B(1) IS KNOWN, THE SECOND EQUATION BECOMES
C             A(1)+E(1)=YI-0.5*Q*Q*D(1). DURING THE SOLUTION OF
C             THE 3N-4 EQUATIONS,A1 WILL BE KEPT IN CELL C(2)
C             INSTEAD OF C(1) TO RETAIN THE TRIDIAGONAL FORM OF THE
C             COEFFICIENT MATRIX.
C     ------------------------------------------------------------------
    5 C(2)=0.0
      W(2)=0.5*Q*Q*D(1)
   10 M=N-2
      IF (M.LE.0) GO TO 20
C     ------------------------------------------------------------------
C             UPPER TRIANGULARIZATION OF THE TRIDIAGONAL SYSTEM OF
C             EQUATIONS FOR THE COEFFICIENT MATRIX FOLLOWS--
C     ------------------------------------------------------------------
      DO 15 I=1,M
      AI=Q
      Q=X(I+2)-X(I+1)
      H=AI/Q
      C(3*I)=-H/(2.0-C(3*I-1))
      W(3*I)=(-YI-W(3*I-1))/(2.0-C(3*I-1))
      C(3*I+1)=-H*H/(H-C(3*I))
      W(3*I+1)=(YI-W(3*I))/(H-C(3*I))
      YI=Y(I+2)-Y(I+1)
      C(3*I+2)=1.0/(1.0-C(3*I+1))
   15 W(3*I+2)=(YI-W(3*I+1))/(1.0-C(3*I+1))
C     ------------------------------------------------------------------
C             E(N-1) IS DETERMINED DIRECTLY FROM THE LAST EQUATION
C             OBTAINED ABOVE, AND THE FIRST OR SECOND DERIVATIVE
C             VALUE GIVEN AT THE END POINT.
C     ------------------------------------------------------------------
   20 IF (J.EQ.1) GO TO 25
      C(3*N-3)=(Q*Q*D(2)/2.0-W(3*N-4))/(3.0-C(3*N-4))
      GO TO 30
   25 C(3*N-3)=(Q*D(2)-YI-W(3*N-4))/(2.0-C(3*N-4))
   30 M=3*N-6
      IF (M.LE.0) GO TO 40
C     ------------------------------------------------------------------
C             BACK SOLUTION FOR ALL COEFFICENTS EXCEPT
C             A(1) AND B(1) FOLLOWS--
C     ------------------------------------------------------------------
      DO 35 II=1,M
      I=M-II+3
   35 C(I)=W(I)-C(I)*C(I+1)
   40 IF (J.EQ.1) GO TO 45
C     -----------------------------------------------------------------
C
C                IF THE SECOND DERIVATIVE IS GIVEN AT THE END POINTS,
C                A(1) CAN NOW BE COMPUTED FROM THE KNOWN VALUES OF
C                B(1) AND E(1). THEN A(1) AND B(1) ARE PUT INTO THEIR
C                PROPER PLACES IN THE C ARRAY.
C     -----------------------------------------------------------------
      C(1)=Y(2)-Y(1)-W(2)-C(3)
      C(2)=W(2)
      RETURN
   45 C(2)=W(2)-C(3)
      RETURN
      END
```

SUBROUTINE SPLNB

```
      SUBROUTINE SPLNB (N,X,Y,C,V)
      DIMENSION X(10), Y(10), C(30), V(5)
      V(5)=2.0
      LIM=N-1
C                   -----------------------------------------------------
C                   DETERMINE IN WHICH INTERVAL THE INDEPENDENT
C                   VARIABLE,V(1),LIES.
C                   -----------------------------------------------------
      DO 5 I=2,LIM
      IF (V(1).LT.X(I)) GO TO 10
    5 CONTINUE
      I=N
      IF (V(1).GT.X(N)) V(5)=3.0
      GO TO 15
   10 IF (V(1).LT.X(1)) V(5)=1.0
C                   -----------------------------------------------------
C                   Q IS THE SIZE OF THE INTERVAL CONTAINING V(1).
C                   -----------------------------------------------------
C                   Z IS A LINEAR TRANSFORMATION OF THE INTERVAL
C                   ONTO (0,1) AND IS THE VARIABLE FOR WHICH
C                   THE COEFFICIENTS WERE COMPUTED BY SPLNA.
C                   -----------------------------------------------------
   15 Q=X(I)-X(I-1)
      Z=(V(1)-X(I-1))/Q
      V(2)=((Z*C(3*I-3)+C(3*I-4))*Z+C(3*I-5))*Z+Y(I-1)
      V(3)=((3.*Z*C(3*I-3)+2.0*C(3*I-4))*Z+C(3*I-5))/Q
      V(4)=(6.*Z*C(3*I-3)+2.0*C(3*I-4))/(Q*Q)
      RETURN
      END
```

FUNCTION CLOCK

```
      FUNCTION CLOCK (T1,IINC)
C
C    ****    ADD A TIME IN MINUTES TO A 2400 HOUR TIME AND RETURN A 2400
C    ****    HOUR TIME
C
      T2=IINC
      I100=T1/100
      T3=T1-100.0*I100+T2
      I100=I100+INT(T3/60)
      CLOCK=I100*100.0+T3-60.0*INT(T3/60)
      RETURN
      END
```

SUBROUTINE RLINE

```
      SUBROUTINE RLINE (NC,F,KS1,JS)
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSTRT,DTIM,Z1,Z2,DCON,EHC,EXN,F
     1LST,TLST,NSPAR
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICZ,DIGZ,CHRZ
      DIMENSION R(20), F(21), YP(12), TMP(12), OE(20), XNE(20)
      EQUIVALENCE (NR,NRTO), (RTO,R)
      INTEGER PLSP
      RLBK(A,B1,B2,B3)=A*(B1-B2)/(B3-B2)
      IFG=0
      KFACT=KS1-6+JS
      IF (NC.EQ.1) KFACT=KFACT+2
      KS=MAX0(KFACT/MR,0)
      KS=MIN0(KS,NC)
      KSS=MAX0(KFACT-KS*MR,0)
      KS=KS+1
      IF (KS.GT.NC.AND.KSS.EQ.2) GO TO 5
      IF (INFO.EQ.0) WRITE (IOUT,365) PLSP
      IF (INFO.LT.0) WRITE (IOUT,370) PLSP
    5 DO 15 J=1,NL
      M=J
      DO 10 L=J,NL
   10 IF (OZP(L).LT.OZP(M)) M=L
      IF (M.EQ.J) GO TO 15
      SV=OZP(J)
      OZP(J)=OZP(M)
      OZP(M)=SV
   15 CONTINUE
      NR=NC
      NSHC=0
      NSXN=0
      KK=0
      MR1=MR-1
      INX=1
      NCR=(NR+1)/2
      TOL=1.0-(0.17/(SQRT(FLOAT(NR))))
      KSN=KS1+1
      IF (KSN.GT.7) GO TO 40
      GO TO (20,25,30,35,40,40,40),KSN
C     DO CORNERS.
   20 CALL SIM (0.,0.,OC(1),INX)
   25 CALL SIM (0.,XN,OC(2),INX)
   30 IF (KS.EQ.1) CALL SIM (HC,XN,OZN(MR,1),INX)
      OC(3)=OZN(MR,1)
   35 CALL SIM (HC,0.,OC(4),INX)
   40 DO 45 LS=1,NL
      IF (OC(1).LT.OZP(LS)) GO TO 50
   45 CONTINUE
      WRITE (IOUT,355) PLSP,OC(1)
      STOP
   50 IF (LS.GT.1) WRITE (IOUT,360) PLSP,OZP(LS)
      IF (OZP(LS).GT.OC(3)) GO TO 345
      NCYC=0
C     DO DOUBLE ROLLBACK ON EDGES
      OZS=OZP(LS)*0.9
      IF (KSN.GE.7) GO TO 75
      HCG=RLBK (HC,OZS,OC(2),OC(3))
      XNG=RLBK(XN,OZP(LS),OC(4),OC(3))
      IF (HCG.LE.0.) HCG=HC/20.
      IF (XNG.LE.0.) XNG=XN/10.
      IF (XNG.GT.XN) XNG=XN/20.
      IF (NCR.EQ.1) GO TO 90
      GO TO (55,55,55,55,55,65,75),KSN
   55 OS(1)=OZS
```

```
      INX=-1
   60 CALL SIM (HCG,XN,OS(1),INX)
      OHC=OS(1)
      IF (INX.NE.-1) GO TO 65
      HCG1=RLBK (HCG,OZS,OC(2),OS(1))
      AH=HCG1-HCG
      BH=RLBK(HC-HCG,OZS,OS(1),OC(3))
      HCG=HCG+(ABS(AH)*BH+ABS(BH)*AH)/(ABS(AH)+ABS(BH))
      IF (OS(1).GE.OC(3)) HCG=RLBK(HCG,OZS,OC(2),OC(3))
      HCG=AMIN1(HCG,0.5*HC)
      OS(1)=OZS
      IFG=IFG+1
      IF (IFG.EQ.4) INX=1
      GO TO 60
   65 OS(2)=OZP(LS)
      INX=-1
   70 CALL SIM (HC,XNG,OS(2),INX)
      OXN=OS(2)
      IF (INX.NE.-1) GO TO 75
      XNG1=RLBK(XNG,OZP(LS),OC(4),OS(2))
      IF (XNG1.GT.0.5*XN) XNG=XN/3.
      IF (XNG1.LE.0.5*XN) XNG=(RLBK(XN-XNG,OZP(LS),OS(2),OC(3))+XNG+XNG1
     1)/2.
      INX=1
      GO TO 70
   75 IF (KS.GT.NR.AND.KSS.EQ.2) GO TO 245
      IF (KS.GT.NR.AND.KSS.EQ.1) GO TO 80
      AH1=RLBK(HCG,OZS,OC(2),OS(1))-HCG
      BH1=RLBK(HC-HCG,OZS,OS(1),OC(3))
      HCS=HCG+(ABS(AH1)*BH1+ABS(BH1)*AH1)/(ABS(AH1)+ABS(BH1))
      IF (HCS.LE.0.) HCS=HCG
   80 XNS=RLBK(XNG,OZP(LS),OC(4),OS(2))
      IF (XNS.GT.XNG) XNS=RLBK(XN-XNG,OZP(LS),OS(2),OC(3))+XNG
      IF (KS.GT.NR) GO TO 245
      IF (KS.GT.NCR) XSS=XNS
      IF (KS.GT.NCR) OSS=OS(2)
      IF (KS.LT.2) GO TO 90
      IF (KS.EQ.2) GO TO 85
      HTT1=RHO(MR,KS-2)*R(KS-2)/F(KS-2)
      XNN1=RHO(MR,KS-2)/F(KS-2)
   85 HTT=RHO(MR,KS-1)*R(KS-1)/F(KS-1)
      XNN=RHO(MR,KS-1)/F(KS-1)
      IF (KSS.EQ.0) GO TO 90
      HCC=RHO(MR,KS)*R(KS)/F(KS)
      XNX=RHO(MR,KS)/F(KS)
      GO TO 95
   90 XNX=XN
   95 XNX1=0.
      ICNT=KS-1
      DO 240 I=KS,NR
      ICNT=ICNT+1
      IF (I.GT.1) GO TO 100
      HTT=HC
      XNN=XN
      IF (KSS) 175,165,175
  100 IF (I-NCR-1) 105,125,130
  105 OZC=OZN(MR,I-1)*(OZS/OZN(MR,I-1))**(1./FLOAT(NCR+1-I))
      IF (KSS.NE.0) GO TO 120
      HSS=HCS
      OSS=OZS
      IF (OS(1).GT.OZC) HSS=0.
      IF (OS(1).GT.OZC) OSS=OC(2)
      IF (ICNT.GT.2) GO TO 110
      HCC=RLEK(HTT-HSS,OZC,OSS,OZN(MR,I-1))+HSS
      IF (OC(3).GT.OZP(NL)) JJ=NCR-2
      IF (OC(3).LE.OZP(NL)) JJ=NCR-1
      IF (JJ.EQ.0) GO TO 120
      HCC1=HC-(HC-HCS)/FLOAT(JJ)
      HCC=AMAX1(HCC,HCC1)
      GO TO 120
```

```
110 HCC=HTT1-RLBK(HTT1-HTT,OZC,OZN(MR,I-2),OZN(MR,I-1))
    A=RLBK(HTT-HSS,OZC,OSS,OZN(MR,I-1))+HSS
    BX=HTT-HCC
    AX=A-HCS
    IF (OC(3)-OZN(MR,2).GT.0) GO TO 115
    AX=0.
    BX=1.
115 HCC=(HCC*AX+A*BX)/(AX+BX)
    HCC1=HTT-(HTT-HCS)/AMAX0(NCR-I,1)
    HCC=AMAX1(HCC,HCC1)
120 IF (HCC.GT.TOL*HTT) HCC=TOL*HTT
    HMR4=HC-(FLOAT(I-1)*HC/FLOAT(NCR-1))
    IF (HCC.LT.HMR4) HCC=HMR4
    HTT1=HTT
    HTT=HCC
    XNN=XN
    IF (KSS) 175,155,175
125 OZC=OC(3)*(OZP(LS)/OC(3))**(1./FLOAT(NCR))
    XNN=XN
    OZL=OC(3)
    OSS=OZP(LS)
    XSS=XNS
    ICNT=0
    IF (KSS) 150,140,150
130 OZC=OZN(MR,I-1)*(OZP(LS)/OZN(MR,I-1))**(1./FLOAT(NR+2-I))
    OZL=OZN(MR,I-1)
    IF (KS.LE.NCR) GO TO 135
    ICNT=KS-NCR-1
135 ICNT=ICNT+1
    IF (KSS.NE.0) GO TO 150
    IF (ICNT.LE.2) GO TO 140
    XNX1=XNN1-RLBK(XNN1-XNN,OZC,OZN(MR,I-2),OZN(MR,I-1))
140 IF (XNN.GT.XSS) GO TO 145
    XSS=0.
    OSS=OC(4)
    XNS=XNS*0.5
145 XNX=RLBK(XNN-XSS,OZC,OSS,OZL)+XSS
    IF (XNX1.GT.0.0.AND.XNX1.LT.XN) XNX=(XNX+XNX1)/2.0
    IF (OC(3).GT.OZP(NL)) L=1
    IF (OC(3).LE.OZP(NL)) L=2
    IF (NCR.GT.2) XNX=AMAX1(XNX,XNN-(XNN-XNS)/FLOAT(NR+L-I))
    IF (I.LE.NCR+1) GO TO 146
    IF (OC(3).LT.OZN(MR,NCR+1)) XNX=XNN-(XNN-XNS)/FLOAT(NR-I+2)
    IF (OC(3).GT.OZN(MR,NCR+1).AND.I.EQ.NR) XNX=(XNN+2.0*XNS)/3.0
146 CONTINUE
    IF (I.EQ.NR.AND.XNX.LE.0.) XNX=XNN/2.
    IF (NCR.LE.2) XNX=XN/3.0
    IF (XNX.LT.1.1*XNG.AND.XNX.GT.0.9*XNG) XNX=XNG
150 IF (XNX.GT.TOL*XNN) XNX=TOL*XNN
    IF (XNX.GT.XN.OR.OZP(LS).LT.OC(4)) XNX=(XN*FLOAT(NR-I)/FLOAT(NCR-1
   1))
    IF (XNX.LE.0.) XNX=1.0E-7
    XNN1=XNN
    XNN=XNX
    HTT=HC
    IF (KSS.NE.0) GO TO 175
155 IF (OZN(MR,I-1).GT.1.1*OZP(LS)) GO TO 165
    IF (IABS(NCR-I).LE.2) GO TO 165
    GAP=0.
    NCOUNT=I-2
    IF (I.LE.(NR/2+1)) NSTART=1
    IF (I.GT.(NR/2+1)) NSTART=NR/2+1
    DO 160 JJ=NSTART,NCOUNT
    GAP1=OZN(MR,JJ)-OZN(MR,JJ+1)
    IF (GAP1.LT.GAP) GO TO 160
    GAP=GAP1
    HTT=((R(JJ)*RHO(MR,JJ))/F(JJ)+(R(JJ+1)*RHO(MR,JJ+1))/F(JJ+1))/2.0
    XNN=HTT/((R(JJ)+R(JJ+1))/2.)
160 CONTINUE
165 R(I)=HTT/XNN
```

```
      F(I)=SQRT(R(I)*R(I)+1.)
      RHO(MR,I)=XNN*F(I)
      IF (XNX.EQ.XNG) OZN(MR,I)=OS(2)
      IF (OZP(LS).GE.OC(4)) GO TO 169
      IF (I.NE.NR) GO TO 169
      XNLL(MR)=HC
      GO TO 170
  169 CONTINUE
      IF (I.EQ.1.OR.XNX.EQ.XNG) GO TO 175
      IF (I.EQ.NCR.AND.OZP(LS).GE.OC(2)) INX=-3
      IF (INX.NE.-3) GO TO 171
      ITAPE=NR
      CALL EDGMX(RHO(1,I-1),OZN(1,I-1),MR,HMX,OZHX,LX)
      OZN(MR,I)=OZP(LS)*OZN(MR,I-1)/OZHX
      IF (MR.EQ.LX+1) OZN(MR,I)=OZP(LS)/TOL
      OZR=OZN(MR,I)
  171 CONTINUE
      IF (OZP(LS).GE.OC(2)) GO TO 170
      IF (I.NE.NCR) GO TO 170
      R(I)=0.
      F(I)=1.
      RHO(MR,I)=XN
      HTT=0.
      HCLL(MR)=XN
      XNN=XN
  170 CALL SIM (HTT,XNN,OZN(MR,I),INX)
      IF (INX.GT.0) GO TO 175
      HTT2=RLBK(HTT1-HTT,OZR,OZN(MR,I),OZN(MR,I-1))+HTT
      HTT=AMIN1(HTT2,TOL*HTT1)
      R(I)=HTT/XNN
      F(I)=SQRT(R(I)*R(I)+1.)
      RHO(MR,I)=XNN*F(I)
      INX=1
      GO TO 170
  175 IF (KSS.EQ.0) KSS1=2
      IF (KSS.NE.0) KSS1=KSS+1
      IF (MR1) 240,240,180
  180 IF (MR.EQ.2) GO TO 200
      IF (KSS1.GT.MR1) GO TO 195
      DO 190 J=KSS1,MR1
      K=MR-J+1
      OZC=OZN(K+1,I)*(OZP(LS)/OZN(K+1,I))**(1./FLOAT(K))
      IF (K.EQ.MR1) GO TO 185
      RHO1=RHO(K+2,I)-RLBK(RHO(K+2,I)-RHO(K+1,I),OZC,OZN(K+2,I),OZN(K+1,
     1I))
  185 RHO(K,I)=RLBK(RHO(K+1,I),OZC,OC(1),OZN(K+1,I))
      IF (K.EQ.MR1) RHO1=RHO(K,I)
      IF (RHO1.GT.0.) RHO(K,I)=(RHO1+RHO(K,I))/2.0
      FK=AMAX0(K-2,2)
      RHO(K,I)=AMAX1(RHO(K,I),RHO(K+1,I)-(RHO(K+1,I)/FK))
      IF (RHO(K,I).GE.RHO(K+1,I)) RHO(K,I)=RHO(K+1,I)-(RHO(K+1,I)/FK)
      IF (RHO(K,I).LE.0.) RHO(K,I)=RHO(K+1,I)*0.5
      RHO(K,I)=AMIN1(RHO(K,I),RHO(MR,I)*FLOAT(K)/FLOAT(MR))
      XNX=RHO(K,I)/F(I)
      HCC=R(I)*XNX
      IF (I.EQ.NCR.AND.OZP(LS).LT.OC(2)) HCLL(K)=XNX
      IF (I.EQ.NR.AND.OZP(LS).LT.OC(4)) XNLL(K)=HCC
      CALL SIM (HCC,XNX,OZN(K,I),INX)
  190 CONTINUE
  195 IF (OZN(2,I).LT.OZP(LS)) RHO(1,I)=0.9*RHO(2,I)
      IF (OZN(2,I).LT.OZP(LS)) GO TO 215
  200 OZN(1,I)=OC(1)
      SX=-SIG*3.
      IT=1
      RHO(1,I)=0.
      CALL EDGMX (RHO(1,I),OZN(1,I),MR,HMX,OZHX,LX)
      MM=LX+1
  205 RHO(1,I)=0.
      CALL CURV1 (MM,OZN(1,I),RHO(1,I),SP1,SP2,YP,TMP,SX)
      RHO(1,I)=CURV2(OZP(LS),MM,OZN(1,I),RHO(1,I),YP,SX,IT)
      INX=-2
      IF (IT.GT.0) GO TO 210
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 205
  210 IF (RHO(1,I).GT.0.9*RHO(2,I)) RHO(1,I)=0.9*RHO(2,I)
      IF (RHO(1,I).LE.0.) RHO(1,I)=.5*RHO(2,I)
      IF (RHO(1,I).GE.RHO(2,I)) RHO(1,I)=0.5*RHO(2,I)
      IF (RHO(1,I).LE.0.) RHO(1,I)=RHO(2,I)*0.5
  215 XNX=RHO(1,I)/F(I)
      HCC=XNX*R(I)
      OZN(1,I)=OZP(LS)
      IF (OZP(LS).LT.OC(2).AND.I.EQ.NCR) HCLL(1)=XNX
      IF (I.EQ.NR.AND.OZP(LS).LT.OC(4)) XNLL(1)=HCC
      CALL SIM (HCC,XNX,OZN(1,I),INX)
      IF (INX.NE.-2) GO TO 235
      AH=RLBK(RHO(1,I),OZP(LS),OC(1),OZN(1,I))-RHO(1,I)
      BH=RLBK((RHO(2,I)-RHO(1,I)),OZP(LS),OZN(1,I),OZN(2,I))
      RHO(1,I)=RHO(1,I)+(ABS(AH)*BH+ABS(BH)*AH)/(ABS(AH)+ABS(BH))
      RHO(1,I)=AMIN1(RHO(1,I),0.9*RHO(2,I))
      IF(RHO(1,I).LE.0.) RHO(1,I)=0.5*RHO(2,I)
      IF (I.EQ.NCR) IFG=IFG+1
      IF (IFG.LT.3.AND.I.EQ.NCR) GO TO 215
  230 INX=1
      GO TO 215
  235 KSS=0
  240 CONTINUE
C  CHECK FOR INCREASING RATIOS
  245 DO 260 I=1,NR
      K=I
      DO 250 J=I,NR
  250 IF (R(J).LT.R(K)) K=J
      IF (K.EQ.I) GO TO 260
      SV=R(I)
      R(I)=R(K)
      R(K)=SV
      SV=F(I)
      F(I)=F(K)
      F(K)=SV
      DO 255 J=1,MR
      SV=OZN(J,I)
      OZN(J,I)=OZN(J,K)
      OZN(J,K)=SV
      SV=RHO(J,I)
      RHO(J,I)=RHO(J,K)
  255 RHO(J,K)=SV
  260 CONTINUE
C  DO SPECIAL CALCULATIONS
      KSS1=KSS+1
      IF (OZP(LS).LT.OC(2)) NCR1=NCR-1
      IF (OZP(LS).GE.OC(2)) NCR1=NCR
      NN=NCR1+1
      SX=-20.*SIG/FLOAT(NN)
      IF (NCR.NE.1) GO TO 265
      OT(1)=OC(2)
      HCT(1)=0.
      OT(2)=OHC
      HCT(2)=HCG
      OT(3)=OC(3)
      HCT(3)=HC
      III=0
      NN=3
      GO TO 295
  265 DO 270 I=1,NCR1
      IF (OZP(LS).LT.OC(2)) L=I+1
      IF (OZP(LS).GE.OC(2)) L=I
      OT(I+2)=OZN(MR,L)
  270 HCT(I+2)=RHO(MR,L)*R(L)/F(L)
      OT(1)=OC(2)
      HCT(1)=0.
      OT(2)=OHC
      HCT(2)=HCG
      NN=NN+1
      IF (KSS1.GT.1) GO TO 300
      IF (HCG.GT.TOL*HCT(3)) HCS=TOL*HCT(3)
      IF (HCS.EQ.TOL*HCT(3)) GO TO 295
      IT=1
  275 CALL CURV1 (NN,OT,HCT,SP1,SP2,YP,TMP,SX)
      DO 280 LK=1,NL
      IF (OZP(LK).GE.OC(2)) GO TO 285
  280 CONTINUE
      LK=NL
  285 OZS=OZP(LK)*0.7
      HCS=CURV2(OZS,NN,OT,HCT,YP,SX,IT)
      IF (IT.GT.0) GO TO 290
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 275
  290 IF (HCS.GT.TOL*HCT(3)) HCS=TOL*HCT(3)
  295 IF (NCR.EQ.1) HCS=HC/3.
      IF (HCS.GE.HCT(3).OR.HCS.LE.HCT(1)) HCS=(HCT(1)+HCT(3))/2.
      CALL SIM (HCS,XN,OS(1),INX)
  300 OT(2)=OS(1)
      HCT(2)=HCS
      NT=NN
      IF (KSS1.GT.2) GO TO 340
      SX=-SIG*20./FLOAT(NN)
      XNN=HC/RTO(NR)
      IF (NCR.EQ.1) GO TO 335
      IF (OZN(MR,NR).LT.1.1*OZP(LS)) XNS=XNN*0.5
      IF (OC(4).GT.OZP(LS)) XNS=XNN*0.5
      IF (XNS.EQ.XNN*0.5) GO TO 335
      NCR1=NCR
      IF (OZP(LS).LT.OC(4)) NCR1=NCR-1
      DO 305 I=1,NCR1
      J=NR+1-I
      IF (OZP(LS).LT.OC(4)) J=J+1
      OE(I+1)=OZN(MR,J)
  305 XNE(I+1)=RHO(MR,J)/F(J)
      OE(1)=OC(4)
      XNE(1)=0.
      NN=NCR1+1
  310 IF (OE(NN).LT.OE(NN-1)) NN=NN-1
      IF (NN.EQ.1) XNS=XNN*0.5
      IF (NN.EQ.1) GO TO 335
      IF (OE(NN).LT.OE(NN-1)) GO TO 310
      IF (XNG.GE.XNE(2)) GO TO 320
      IF (ABS(XNE(2)-XNG).LT..0001) GO TO 325
      NN=NN+1
      NNR=NN-2
      DO 315 I=1,NNR
      II=NN-I+1
      XNE(II)=XNE(II-1)
  315 OE(II)=OE(II-1)
      XNE(2)=XNG
      OE(2)=OXN
      SX=-SIG*20./FLOAT(NN)
  320 IT=1
  325 CALL CURV1 (NN,OE,XNE,SP1,SP2,YP,TMP,SX)
      DO 326 LK=LS,NL
      IF (OZP(LK).GE.OC(4)) GO TO 327
  326 CONTINUE
      LK=NL
  327 XNS=CURV2(OZP(LK),NN,OE,XNE,YP,SX,IT)
      IF (IT.GT.0) GO TO 330
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 325
  330 IF (XNS.GT.TOL*XNE(2)) XNS=TOL*XNE(2)
      IF (XNS.GE.XNE(3).OR.XNS.LE.XNE(1)) XNS=(XNE(1)+XNE(3))/2.
  335 IF (NCR.EQ.1) XNS=XN/3.
      CALL SIM (HC,XNS,OS(2),INX)
  340 RETURN
  345 WRITE (IOUT,350) PLSP
      STOP
C
C
C
  350 FORMAT (1H1,11HTHE LOWEST ,A4,24H LINE CANNOT BE PLOTTED./1H0,39HI
     1NCREASE THE MAXIMUM HC AND NOX VALUES.)
  355 FORMAT (1H1,24HNO LINES CAN BE PLOTTED./1H0,35HBACKGROUND ONLY PRO
     1DUCES TOO MUCH  ,A4,1H,,F5.2,5H PPM.)
  360 FORMAT (1H0,45HDUE TO HIGH BACKGROUND CONDITIONS THE LOWEST ,A4,17
     1H PLOTTED WILL BE ,F5.2,5H PPM.)
  365 FORMAT (1H1,//,14X,36HTHE FOLLOWING SIMULATIONS WERE DONE./1H0/1H
     1,16X,2HHC,18X,3HNOX,15X,5HRATIO,17X,A4)
  370 FORMAT (1H1,//,14X,36HTHE FOLLOWING SIMULATIONS WERE DONE./1H0/1H
     1,16X,2HHC,18X,3HNOX,15X,5HRATIO,17X,A4,16X,4HTIME)
      END
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SUBROUTINE SIM

```
      SUBROUTINE SIM (HC,XN,ZN,INX)
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /TITL/ ITTL(18)
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FEX(2),CI(81),REACT(81),NI,PLSP
      COMMON /INOUT/ INP,IOUT,ITAPE
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KPH(9)
      COMMON /SUNLIT/ XJ(47,10),SIGGA(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(016),XZ(016),KJ(16),JSTRT,JSTOP,SPEE(11),MNLM(11),MXLM(11),MAXL
     3,MAXJ
      COMMON /MIX/ NMIX,AMIX(16),STRM,STOPM,DC(45),TSTART
      COMMON /SUPPR/NOPR
      COMMON /SURFAC/FINALD(4)
      DIMENSION RT(200), RX(9), C(81)
      DIMENSION ISPN(2)
      INTEGER REACT,SPECIS,PLSP
      DATA ISPN/'NO2 ','O3  '/
      TCI=FLOAT(JSTRT)
      START=0.
      T=START
      TDIL=0.
      IF (NSPARS.EQ.1) SAV=STOPP
      STOPP=SAV
      FLST=1.0
      TLST=START
      EHC=HC
      EXN=XN
      IF (NPTO.EQ.0) TPRNT=STOPP
      IF (NPTO.NE.0) TM=5.0
      IF (NPTO.NE.0) CALL ISOPLT (HC,XN)
      H=1.E-10
      N=NI
      M=NS-1
      DO 5 I=1,N
    5 C(I)=CI(I)
      CALL RATES (C,N)
      IF (NSPARS.NE.0) CALL SPARS (IA,JA,M)
      DO 10 J=1,NHC
      K=IH(J)
      C(K)=(HC*RCTY(J)+HCIN*FINHC(J))/CARB(J)
   10 CONTINUE
      IF (NALD.EQ.0) GO TO 20
      DO 15 J=1,NALD
      K=IALD(J)
      C(K)=(HC*ALDX(J)+HCIN*FINALD(J))/ALDCRB(J)
   15 CONTINUE
   20 DO 25 K=1,2
      I=INOX(K)
      IF (SPECIS(I).EQ.ISPN(1)) C(I)=XN*XNF(K)+XNIN
      IF (SPECIS(I).NE.ISPN(1)) C(I)=XN*XNF(K)
   25 CONTINUE
      IF (OZIN.EQ.0.) GO TO 40
      IF (PLSP.NE.ISPN(2)) GO TO 30
      C(KOZ)=OZIN
      GO TO 40
   30 DO 35 I=1,N
      IF (SPECIS(I).NE.ISPN(2)) GO TO 35
      C(I)=OZIN
      GO TO 40
   35 CONTINUE
   40 CALL DIFSET (N,START,C,RT)
      IF (NPTO.EQ.0) GO TO 50
      WRITE (IOUT,190)
      WRITE (IOUT,200) (ITTL(I),I=1,18)
      IF (INFO.LT.1) WRITE (IOUT,235) PLSP
      IF (INFO.LT.1) GO TO 50
      IF (NI.NE.0) WRITE (IOUT,245) (REACT(I),I=1,NI)
      IF (NI.NE.0) WRITE (IOUT,250) (CI(I),I=1,NI)
      WRITE (IOUT,215) ERR
      WRITE (IOUT,220) (R(IR),IR=1,NR)
      IF (IP.EQ.0) GO TO 50
      DO 45 I=1,IP
      K=IPH(I)
   45 RX(I)=R(K)
      WRITE (IOUT,225) (IPH(IR),IR=1,IP)
      WRITE (IOUT,230) (RX(IR),IR=1,IP)
   50 IN=1
      IF (NSPARS.EQ.0) IN=4
      NSPARS=0
      TNEXT=1.
      IF (NPTO.EQ.0) GO TO 90
      IF (T-START) 115,115,90
   55 IF (AMIX(1).GT.-1..AND.T.GE.TDIL) TDIL=TDIL+60.
      IF (DTIM.EQ.0.) GO TO 85
      IF (T.GE.TSRT) GO TO 70
      IF (TSRT-TPRNT-20.) 60,60,65
   60 TNEXT=TSRT
      IN=2
      GO TO 90
   65 TNEXT=TPRNT
      IN=0
      GO TO 90
   70 IF (AMIX(1).LT.-1.) GO TO 71
      TNEXT=AMIN1(TDIL,TPRNT)
      IF (T.GE.TSRT+DTIM) GO TO 85
      GO TO 74
   71 IF (T.GE.TSRT+DTIM) GO TO 85
      TLST=TSRT
      TNEXT=TSRT+DTIM
   74 IF (TNEXT-TPRNT-20.) 75,75,80
   75 IN=2
      GO TO 90
   80 TNEXT=TPRNT
      IN=0
      GO TO 90
   85 TNEXT=AMIN1(TPRNT,STOPP)
      TLST=TSRT+DTIM
   90 CALL DRIVES (M,T,H,C,TNEXT,ERR,21,IN,IA,JA)
      T=TNEXT
      IF (NPTO.NE.0) GO TO 100
      IF (T.LT.STOPP) GO TO 55
      IF (INX.GT.-1) GO TO 100
      IF (INX.EQ.-1.AND.OZM.GT.0.75*ZN) GO TO 100
      IF (INX.NE.-3) GO TO 91
      TOL=1.0-(0.17/(SQRT(FLOAT(ITAPE))))
      IF (OZM.GE.TOL*ZN.AND.OZM.LE.ZN/TOL) GO TO 100
   91 CONTINUE
      IF (INX.NE.-2) GO TO 95
      IF (OZM.LT.1.1*ZN.AND.OZM.GT.0.9*ZN) GO TO 100
   95 ZN=OZM
      RETURN
  100 ZN=OZM
      IF (NPTO.NE.0) GO TO 110
      INX=1
      IF (T.LT.STOPP) GO TO 55
      IF (XN.EQ.0.) RR=0.
      IF (XN.NE.0.) RR=HC/XN
      IF (INFO.LT.0) GO TO 105
      IF(NOFR.EQ.1) RETURN
      IF (TM.GT.0.) WRITE (IOUT,165) HC,XN,RR,ZN
      IF (TM.LE.0.) WRITE (IOUT,185) HC,XN,RR,ZN
      RETURN
  105 IF (TM.GT.0.) WRITE (IOUT,205) HC,XN,RR,ZN,TM
      IF (TM.LT.0.) WRITE (IOUT,210) HC,XN,RR,ZN
      RETURN
  110 IF (IN.NE.0) RETURN
      IF (T.GE.STOPP) TPRNT=STOPP
      IF (T.LT.TPRNT) GO TO 55
  115 HCC=0.
      DO 120 I=1,NHC
      K=IH(I)
  120 HCC=HCC+CARB(I)*C(K)
      FPROP=0.
      ALDC=0.
      IF (HCC.LT.0.0000001) GO TO 140
      IF (NHC.EQ.0) GO TO 130
      DO 125 I=1,NHC
      K=IH(I)
  125 IF (CARB(I).EQ.3.0) FPROP=3.0*C(K)/HCC
  130 IF (NALD.EQ.0) GO TO 140
      DO 135 I=1,NALD
      K=IALD(I)
  135 ALDC=ALDC+ALDCRB(I)*C(K)
      ALDC=ALDC/HCC
  140 CNOX=0.
      DO 145 I=1,2
      K=INOX(I)
      IF (I.EQ.1) FNO2=C(K)
  145 CNOX=CNOX+C(K)
      IF (CNOX.LE.0.0000001) FNO2=0.
      IF (CNOX.GT.0.0000001) FNO2=FNO2/CNOX
      CO3=C(KOZ)
      IF (INFO.GT.0) WRITE (IOUT,190)
      IF (INFO.GT.0) WRITE (IOUT,235) PLSP
      IF (T.EQ.START) TIMNW=START
      IF (T.NE.START) TIMNW=TPRNT
      CTIME=CLOCK(TCI,IFIX(TIMNW))
      WRITE (IOUT,240) CTIME,HCC,FPROP,ALDC,CNOX,FNO2,CO3
      IF (INFO.LE.0) GO TO 160
      WRITE (IOUT,180) (SPECIS(I),I=1,M)
      WRITE (IOUT,195) CTIME,(C(I),I=1,10),H,(C(I),I=11,M)
      CALL DIFFUN (N,TIMNW,C,RT)
      WRITE (IOUT,170) (RT(I),I=1,M)
      DO 150 I=1,NR
      J=KR(I,1)
      K=KR(I,2)
      L=KR(I,3)
      IF (J.EQ.0) RT(I)=0.
      IF (J.EQ.0) GO TO 150
      IF (J.EQ.99) J=0
      IF (J.EQ.0) TJ=1.
      IF (J.NE.0) TJ=C(J)
      IF (K.EQ.0) TK=1.
      IF (K.NE.0) TK=C(K)
      IF (L.EQ.0) TL=1.
      IF (L.NE.0) TL=C(L)
      RT(I)=TJ*TK*TL*R(I)
  150 CONTINUE
      WRITE (IOUT,175) (RT(I),I=1,NR)
      IF (IP.EQ.0) GO TO 160
      DO 155 I=1,IP
      K=IPH(I)
  155 RX(I)=R(K)
      WRITE (IOUT,230) (RX(I),I=1,IP)
  160 IF (TIMNW.EQ.START) GO TO 90
      IF (NPTO.NE.0) NSPARS=1
      IF (T.GE.STOPP) RETURN
      TPRNT=TPRNT+TSTEP
      GO TO 55
C
C
C
  165 FORMAT (1H0,4F20.5)
  170 FORMAT (/,10H NET RATES,1X,1P10E12.5,/,(11X,1P10E12.5))
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```
175 FORMAT (//,1X,22HTHE REACTICN RATES ARE,/,(1H ,1P10E13.5))
180 FORMAT (//,3X,5HTIME ,4X,10(4X,A4,4X),/,1X,8HINTERVAL,3X,10(4X,A4,
   14X),/,(12X,10(4X,A4,4X)))
185 FORMAT (1H0,4F20.5,8H NOT MAX)
190 FORMAT (1H1///////////)
195 FORMAT (/,1PE11.3,10E12.3/,E11.3,10E12.3/,(11X,10E12.3))
200 FORMAT (46X,18A4)
205 FORMAT (1H0,4F20.5,F21.0)
210 FORMAT (1H0,4F20.5,14X,7HNOT MAX)
215 FORMAT (24H0THE ERROR TOLERANCE IS ,1PE10.3)
220 FORMAT (29H0THE RATE CONSTANTS USED WERE,//,(1H0,1P10E13.3))
225 FORMAT (29H0THE PHOTOLYSIS PEACTIONS ARE,/(1H0,9I13))
230 FORMAT (34H0THE FHOTOLYTIC RATE CONSTANTS ARE,/,(1H0,4X,1P9E13.3))
235 FORMAT (1H0,30X,4HTIME,6X,2HHC,7X,9HFROPYLENE,5X,8HALDEHYDE,6X,3HN
   10X,10X,3HNO2,8X,A4,/,30X,6H(LDT ),4X,5HTOTAL,5X,8HFRACTION,6X,8HFR
   2ACTICN,5X,5HTOTAL,7X,8HFRACTION,3X,9H(INSTANT))
240 FORMAT (1H0,28X,F6.0,1X,F10.5,2X,F10.5,3X,F10.5,1X,F10.5,3X,F10.5,
   12X,F10.5)
245 FORMAT (1H0,22HINITIAL CONCENTRATIONS,//,(12X,10(4X,A4,4X)))
250 FORMAT (/(10X,1P10E12.3))
    END
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SUBROUTINE DRIVES

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      SUBROUTINE DRIVES (N,T0,H0,Y0,TOUT,EPS,MF,INDEX,IA,JA)
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      DIMENSION IA(1), JA(1), Y0(N)
      DIMENSION Y(80,6)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART
      COMMON /GEAR2/ YMAX(100)/GEAR3/ERROR(100)
      COMMON /GEAR5/ IW1(81,9)/GEAR6/W2(1500)/GEAR7/IW2(1500)
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,NZA,NPL,NPU,NZL,NZU,NZRO
      COMMON /INOUT/ INP,LOUT,ITAPE
      DIMENSION W1(80,3)
      DATA NMX/80/,LENW2/1500/,LENIW2/1500/
      NGP=0
      IF (INDEX.EQ.4) GO TO 15
      IF (INDEX.EQ.0) GO TO 30
      IF (INDEX.EQ.2) GO TO 35
      IF (INDEX.EQ.-1) GO TO 40
      IF (INDEX.EQ.3) GO TO 45
      IF (INDEX.NE.1) GO TO 125
      IF (EPS.LE.0.) GO TO 110
      IF (N.LE.0) GO TO 115
      IF ((T0-TOUT)*H0.GE.0.) GO TO 120
      MITER=MF-10*(MF/10)
      IF ((MITER.NE.1).AND.(MITER.NE.2)) GO TO 15
      NP1=N+1
      NZA=IA(NP1)-1
      MAX=LENIW2/2
      IPTI2=MAX+1
      CALL SORDER (N,IA,JA,IW1,IW1(1,5),MAX,IW2,IW2(IPTI2),IER)
      IPTI2=NZA+1
      IF (IPTI2+NZA-1.GT.LENIW2) GO TO 135
      DO 5 I=1,NP1
    5 IW1(I,2)=IA(I)
      DO 10 I=1,NZA
   10 IW2(I)=JA(I)
      CALL NSCORD (N,IW1(1,2),IW2,IW1(1,3),IW2(IPTI2),IW1,IW1(1,5),IW1(1
     1,8))
      MAXPL=(LENIW2-NZA)/2
      IPTI3=IPTI2+MAXPL
      MAXPU=LENIW2-IPTI3+1
      CALL NSSFAC (N,IW1(1,2),IW2,MAXPL,IW1(1,3),IW2(IPTI2),IW1(1,4),MAX
     1PU,IW1(1,5),IW2(IPTI3),IW1(1,6),IW1(1,7),IW1(1,8),IER)
      NPL=IW1(N,4)
      NPU=IW1(N,6)
      NZL=IW1(N+1,3)
      NZU=IW1(N+1,5)
      IPTR2=NZA+1
      IPTR3=IPTR2+MAX0(NZA,NZL)
      IF (IPTR3+MAX0(NZA,NZU)-1.GT.LENW2) GO TO 135
   15 DO 20 I=1,N
      YMAX(I)=ABS(Y0(I))
      IF (YMAX(I).EQ.0.) YMAX(I)=1.E-10
   20 Y(I,1)=Y0(I)
      NC=N
      T=T0
      H=H0
      NZRO=0
      TST=EPS*1.E-10
      DO 25 I=1,N
   25 IF (Y(I,1).GT.TST) NZRO=NZRO+1
      NZRO=MAX0(NZRO,1)
      NOLD=NZRO
      HMIN=ABS(H0)
      HMAX=ABS(T0-TOUT)*10.
      HMAX=AMIN1(HMAX,20.)
      EPSC=EPS
      MFC=MF
      JSTART=0
      NO=N
      CALL OZMX (Y,TL,TOUT,NO)
      NMX1=NMX+1
      EPSJ=SQRT(UROUND)
      NHCUT=0
      GO TO 50
   30 HMAX=ABS(TOUT-TOUTP)*10.
      HMAX=AMIN1(HMAX,20.)
      GO TO 70
   35 HMAX=ABS(TOUT-TOUTP)*10.
      HMAX=AMIN1(HMAX,20.)
      IF ((T-TOUT)*H.GE.0.) GO TO 140
      GO TO 75
   40 IF ((T-TOUT)*H.GE.0.) GO TO 130
      JSTART=-1
      NC=N
      EPSC=EPS
      MFC=MF
   45 CONTINUE
   50 CALL STIFFS (Y,NO,IA,JA,W1,NMX,IW1,NMX1)
      IF (NPTO.NE.0) CALL SAVLIN (T,Y(KOZ,1))
      KGO=1-KFLAG
      GO TO (55,85,100,90),KGO
   55 CONTINUE
      IF (T.GE.TL) CALL OZMX (Y,TL,TOUT,NO)
      D=0.
      NZRO=0
      DO 65 I=1,NC
      IF (Y(I,1).GE.0.) GO TO 60
      NGP=NGP+1
      DO 56 J=1,6
   56 Y(I,J)=0.
   60 CONTINUE
      IF (Y(I,1).GT.TST) NZRO=NZRO+1
      AYI=ABS(Y(I,1))
      YMAX(I)=AMAX1(1.E-10,AYI)
   65 D=D+(AYI/YMAX(I))**2
      NZRO=MAX0(NZRO,1)
      IF (NZRO.NE.NOLD) JSTART=-1
      D=D*(UROUND/EPS)**2
      IF (D.GT.FLOAT(N)) GO TO 105
      IF (INDEX.EQ.3) GO TO 140
      IF (INDEX.EQ.2) GO TO 75
   70 IF ((T-TOUT)*H.LT.0.) GO TO 45
      CALL INTERP (TOUT,Y,NO,Y0)
      GO TO 150
   75 IF (T.GE.TOUT) GO TO 80
      IF (((T+H)-TOUT).LE.0.) GO TO 45
      H=(TOUT-T)*(1.+4.*UROUND)
      JSTART=-1
      GO TO 45
   80 JSTART=-1
      H=AMIN1(H,1.)
      GO TO 140
   85 CONTINUE
   90 IF (NHCUT.EQ.10) GO TO 95
      NHCUT=NHCUT+1
      HMIN=.1*HMIN
      H=.1*H
      JSTART=-1
      GO TO 45
   95 WRITE (LOUT,155)
      IF (KGO.EQ.4) WRITE (LOUT,170) T
      STOP
  100 WRITE (LOUT,160) T,H
      STOP
  105 WRITE (LOUT,165) T
      KFLAG=-2
      STOP
  110 WRITE (LOUT,175)
      STOP
  115 WRITE (LOUT,180)
      STOP
  120 WRITE (LOUT,185)
      STOP
  125 WRITE (LOUT,190) INDEX
      STOP
  130 WRITE (LOUT,195) T,TOUT,H
      STOP
  135 WRITE (LOUT,200)
      STOP
  140 TOUT=T
      DO 145 I=1,N
  145 Y0(I)=Y(I,1)
  150 INDEX=KFLAG
      TOUTP=TOUT
      H0=HUSED
      IF (KFLAG.NE.0) H0=H
      RETURN
C
C
  155 FORMAT (//44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT//)
  160 FORMAT (//35H KFLAG = -2 FROM INTEGRATOR AT T = ,E16.8,5H  H =,E16
     1.8/52H  THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED//)
  165 FORMAT (//37H INTEGRATION HALTED BY DRIVER AT T = ,E16.8/56H  EPS
     1TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION/)
  170 FORMAT (//35H KFLAG = -3 FROM INTEGRATOR AT T = ,E16.8/45H  CORREC
     1TOR CONVERGENCE COULD NOT BE ACHIEVED/)
  175 FORMAT (//28H ILLEGAL INPUT.. EPS .LE. 0.//)
  180 FORMAT (//25H ILLEGAL INPUT.. N .LE. 0//)
  185 FORMAT (//36H ILLEGAL INPUT.. (T0-TOUT)*H .GE. 0.//)
  190 FORMAT (//24H ILLEGAL INPUT.. INDEX =,I5//)
  195 FORMAT (//44H INDEX = -1 ON INFUT WITH (T-TOUT)*H .GE. 0./4H T =,E
     116.8,9H   TOUT =,E16.8,6H   H =,E16.8)
  200 FORMAT (//42H INSUFFICIENT WORKING STORAGE IN IW2 OR W2//)
      END
```

SUBROUTINE STIFFS

```
      SUBROUTINE STIFFS (Y,NO,IA,JA,W1,NMX,IW1,NMX1)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS,UROUND,N,MF,KFLAG,JSTART
      COMMON /GEAR2/ YMAX(100)/GEAR3/ERROR(100)
      COMMON /GEAR6/ W2(1500)/GEAR7/IW2(1500)
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,IDUMMY(5),NZRO
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IB(80),
     1JB(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      DIMENSION Y(NO,1), IA(1), JA(1), W1(NMX,1), IW1(NMX1,1)
      DIMENSION EL(13), TQ(4), RT(3)
      DATA EL(2)/1./,OLDL0/1./
      KFLAG=0
      TOLD=T
      IF (JSTART.GT.0) GO TO 50
      IF (JSTART.NE.0) GO TO 10
      CALL DIFFUN (N,T,Y,W1)
      DO 5 I=1,N
    5 Y(I,2)=H*W1(I,1)
      METH=MF/10
      MITER=MF-10*METH
      NQ=1
      L=2
      IDOUB=3
      RMAX=1.E4
      RC=0.
      CRATE=1.
      HOLD=H
      MFOLD=MF
      NSTEP=0
      NSTEPJ=0
      NFE=1
      NJE=0
      IRET=3
      GO TO 15
   10 IF (MF.EQ.MFOLD) GO TO 25
      MEO=METH
      MIO=MITER
      METH=MF/10
      MITER=MF-10*METH
      MFOLD=MF
      IF (MITER.NE.MIO) IWEVAL=MITER
      IF (METH.EQ.MEO) GO TO 25
      IDOUB=L+1
      IRET=1
   15 CALL COSET (METH,NQ,EL,TQ,MAXDER)
      LMAX=MAXDER+1
      RC=RC*EL(1)/OLDL0
      OLDL0=EL(1)
   20 FN=FLOAT(NZRO)
      EDN=FN*(TQ(1)*EPS)**2
      E=FN*(TQ(2)*EPS)**2
      EUP=FN*(TQ(3)*EPS)**2
      BND=FN*(TQ(4)*EPS)**2
      EPSOLD=EPS
      NOLD=NZRO
      GO TO (30,35,50),IRET
   25 IF (EPS.EQ.EPSOLD.AND.NZRO.EQ.NOLD) GO TO 30
      IRET=1
      GO TO 20
   30 IF (H.EQ.HOLD) GO TO 50
      RH=H/HOLD
      H=HOLD
      IREDO=3
      GO TO 40
   35 RH=AMAX1(RH,HMIN/ABS(H))
   40 RH=AMIN1(RH,HMAX/ABS(H),RMAX)
      R1=1.
      DO 45 J=2,L
      R1=R1*RH
      DO 45 I=1,N
   45 Y(I,J)=Y(I,J)*R1
      H=H*RH
      RC=RC*RH
      IDOUB=L+1
      IF (IREDO.EQ.0) GO TO 275
   50 IF (ABS(RC-1.).GT.0.3) IWEVAL=MITER
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL=MITER
      T=T+H
      DO 55 J1=1,NQ
      DO 55 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 55 I=1,N
   55 Y(I,J)=Y(I,J)+Y(I,J+1)
   60 DO 65 I=1,N
   65 ERROR(I)=0.
      M=0
      CALL DIFFUN (N,T,Y,W1(1,2))
      NFE=NFE+1
      IF (IWEVAL.LE.0) GO TO 125
      IWEVAL=0
      RC=1.
      NJE=NJE+1
      NSTEPJ=NSTEP
      CON=-H*EL(1)
      ISV=M
      LSV=L
      NZ=IA(N+1)-1
      DO 70 I=1,NZ
   70 W2(I)=0.
      DO 110 IR=1,NR
      IF (KR(IR,1).EQ.0.OR.KR(IR,1).EQ.99) GO TO 110
      MT=ITYPE(IR)
      DO 75 I=1,MT
      JX=I+1-I/3*3
      KX=I+2-I/2*3
      J=KR(IR,JX)
      K=KR(IR,KX)
      IF (J.EQ.0) XX=1.
      IF (J.GT.0) XX=Y(J,1)
      IF (K.EQ.0) XK=1.
      IF (K.GT.0) XK=Y(K,1)
   75 RT(I)=R(IR)*XX*XK
      DO 105 K=1,MT
      I=KR(IR,K)
      DO 85 L=1,MT
      J=KR(IR,L)
      M=IA(J)-1
   80 M=M+1
      IF (I-JA(M)) 80,85,80
   85 W2(M)=W2(M)-RT(L)
      DO 100 L=4,7
      J=KR(IR,L)
      M=IA(I)-1
      IF (J) 100,105,90
   90 M=M+1
      IF (J-JA(M)) 90,95,90
   95 W2(M)=W2(M)+RT(K)
  100 CONTINUE
  105 CONTINUE
  110 CONTINUE
      DO 120 J=1,N
      KMIN=IA(J)
      KMAX=IA(J+1)-1
      DO 115 K=KMIN,KMAX
      W2(K)=W2(K)*CON
      IF (JA(K).EQ.J) W2(K)=W2(K)+1.-CON*DILUT
  115 CONTINUE
  120 CONTINUE
      CALL NSCORA (N,IA,JA,W2,IW1(1,2),W2(IPTR2),IW1,IW1(1,7),IW1(1,8))
      CALL NSNFAC (N,IW1(1,2),IW2,W2,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPT
     1R2),W1(1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1,IW1(1,7),IW1
     2(1,8),IER)
      M=ISV
      L=LSV
      IF (IER.NE.0) GO TO 145
  125 DO 130 I=1,N
      IF (M.LE.0) GO TO 130
      IF (-H*W1(I,2)*10..GT.Y(I,1)) GO TO 140
  130 W1(I,1)=H*W1(I,2)-(Y(I,2)+ERROR(I))
      CALL NSBSLV (N,IW1,IW1,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPTR2),W1(1
     1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1(1,2),W1,W2)
      D=0.
      DO 135 I=1,N
      ERROR(I)=ERROR(I)+W1(I,2)
      D=D+(W1(I,2)/YMAX(I))**2
  135 W1(I,1)=Y(I,1)+EL(1)*ERROR(I)
      IF (M.NE.0) CRATE=AMAX1(.9*CRATE,D/D1)
      IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 160
      D1=D
      M=M+1
      IF (M.EQ.3) GO TO 140
      CALL DIFFUN (N,T,W1,W1(1,2))
      GO TO 125
  140 NFE=NFE+2
      IF (IWEVAL.EQ.-1) GO TO 155
  145 T=TOLD
      RMAX=2.
      DO 150 J1=1,NQ
      DO 150 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 150 I=1,N
  150 Y(I,J)=Y(I,J)-Y(I,J+1)
      IF (ABS(H).LE.HMIN*1.00001) GO TO 270
      RH=.25
      IREDO=1
      GO TO 35
  155 IWEVAL=MITER
      GO TO 60
  160 IF (MITER.NE.0) IWEVAL=-1
      NFE=NFE+M
      D=0.
      DO 165 I=1,N
  165 D=D+(ERROR(I)/YMAX(I))**2
      IF (D.GT.E) GO TO 180
      KFLAG=0
      IREDO=0
      NSTEP=NSTEP+1
      HUSED=H
      NQUSED=NQ
      DO 170 J=1,L
      DO 170 I=1,N
  170 Y(I,J)=Y(I,J)+EL(J)*ERROR(I)
      IF (IDOUB.EQ.1) GO TO 190
      IDOUB=IDOUB-1
      IF (IDOUB.GT.1) GO TO 280
      IF (L.EQ.LMAX) GO TO 280
      DO 175 I=1,N
  175 Y(I,LMAX)=ERROR(I)
      GO TO 280
  180 KFLAG=KFLAG-1
      T=TOLD
      DO 185 J1=1,NQ
      DO 185 J2=J1,NQ
      J=(NQ+J1)-J2
      DO 185 I=1,N
  185 Y(I,J)=Y(I,J)-Y(I,J+1)
      RMAX=2.
      IF (ABS(H).LE.HMIN*1.00001) GO TO 260
      IF (KFLAG.LE.-3) GO TO 250
      IREDO=2
      PR3=1.E+20
      GO TO 200
  190 PR3=1.E+20
      IF (L.EQ.LMAX) GO TO 200
      D1=0.
      DO 195 I=1,N
  195 D1=D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2
      ENQ3=.5/FLOAT(L+1)
      PR3=((D1/EUP)**ENQ3)*1.4+1.4E-6
  200 ENQ2=.5/FLOAT(L)
      PR2=((D/E)**ENQ2)*1.2+1.2E-6
      PR1=1.E+20
      IF (NQ.EQ.1) GO TO 210
      D=0.
      DO 205 I=1,N
  205 D=D+(Y(I,L)/YMAX(I))**2
      ENQ1=.5/FLOAT(NQ)
      PR1=((D/EDN)**ENQ1)*1.3+1.3E-6
  210 IF (PR2.LE.PR3) GO TO 215
      IF (PR3.LT.PR1) GO TO 225
      GO TO 220
  215 IF (PR2.GT.PR1) GO TO 220
      NEWQ=NQ
      RH=1./PR2
      GO TO 240
  220 NEWQ=NQ-1
      RH=1./PR1
      GO TO 240
  225 NEWQ=L
      RH=1./PR3
      IF (RH.LT.1.1) GO TO 235
      DO 230 I=1,N
  230 Y(I,NEWQ+1)=ERROR(I)*EL(L)/FLOAT(L)
      GO TO 245
  235 IDOUB=10
      GO TO 280
  240 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 235
      IF (NEWQ.EQ.NQ) GO TO 35
  245 NQ=NEWQ
      L=NQ+1
      IRET=2
      GO TO 15
  250 IF (KFLAG.EQ.-9) GO TO 265
      RH=10.**KFLAG
      RH=AMAX1(HMIN/ABS(H),RH)
      H=H*RH
      CALL DIFFUN (N,T,Y,W1)
      NFE=NFE+1
      DO 255 I=1,N
  255 Y(I,2)=H*W1(I,1)
      IWEVAL=MITER
      IDOUB=10
      IF (NQ.EQ.1) GO TO 50
      NQ=1
      L=2
      IRET=3
      GO TO 15
  260 KFLAG=-1
      GO TO 280
  265 KFLAG=-2
      GO TO 280
  270 KFLAG=-3
      GO TO 280
  275 RMAX=100.
  280 HOLD=H
      JSTART=NQ
      RETURN
      END
```

SUBROUTINE DIFFUN

```
      SUBROUTINE DIFFUN (L,T,X,XT)
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /SUNLIT/ XJ(47,10),SGGMA(31,10),PHI(31,10),U(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(16),XZ(16),KK(16),JSRT,JSTOP,PSPEC(11),MNLM(11),MXLM(11),MAXL,M
     3AXJ
      COMMON /EMIS/ NEM,EM(16),EMHC(16),EMNOX(16),ESRT(2),ESTOP,ESLP,EHS
     1LP,ENSLP,EC(80),EH(80),EX(80)
      COMMON /MIX/ MMIX,BMIX(16),STRM,STOPM,DC(45),TSTART
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KPH(9)
      COMMON /ALOFT/FALALD(4)
      COMMON /MIXING/ DSTRT,DEND,AMC(5),BMC(5),CMC(5),FD(6),FG(6),
     1AMIX(16),DL,TTMAX,SRISE,SRMIN,DELH,TDIL,NMIX
      DIMENSION XT(L), X(L)
      INTEGER SPECIS,PSPEC
      DIMENSION ISPN(2)
      DATA ISPN/'NO2 ','O3  '/
      N=L
      DILU=0.0
      IF(BMIX(1).GT.0.) GO TO 7
      IF(T.LT.TSRT.OR.T.GT.TSRT+DTIM) GO TO 4
      TT=T+TSTART
      TT=TT-SRISE
      FDT=TT/DL
      IF(FDT.LT.0.0) FDT=0.0
      K=0
    1 K=K+1
      IF(FDT.GE.FD(K).AND.FDT.LT.FD(K+1)) GO TO 2
      IF(K.LT.5) GO TO 1
      IF(FDT.LT.FD(2)) GO TO 6
      FGG=1.0
      FGSLP=0.0
      GO TO 6
    2 CONTINUE
      XFD=FDT-FD(K)
      FGG=((AMC(K)*XFD+BMC(K))*XFD+CMC(K))*XFD+FG(K)
      FGSLP=(3.*AMC(K)*XFD+2.*BMC(K))*XFD+CMC(K)
    6 HT=SRMIN+FGG*DELH
      DILU=(FGSLP*DELH)/(HT*DL)
    4 DILU=AMAX1(DILU,0.)
      IF(T.LT.TSRT) HT=Z1
      IF(T.GT.TSRT+DTIM) HT=Z2
      GO TO 8
    7 IF (BMIX(1).LT.0.) GO TO 5
      IF (T.GE.STOPM) DILU=0.
      IF(T.GE.STOPM) HT=BMIX(MMIX)
      IF (T.GE.STOPM) GO TO 5
      I=IFIX(T/60.+1.99999)
      IF (I.LE.1) I=2
      Z=T-FLOAT(I-2)*60.
      HT=((Z*DC(3*I-3)+DC(3*I-4))*Z+DC(3*I-5))*Z+BMIX(I-1)
      DILU=((Z*3.*DC(3*I-3)+2.*DC(3*I-4))*Z+DC(3*I-5))/HT
    8 CONTINUE
    5 DILUT=AMAX1(DILU,0.)
      DO 10 I=1,N
      XT(I)=-DILUT*X(I)
      IF (SPECIS(I).EQ.ISPN(2)) XT(I)=DILUT*(OZAL-X(I))
   10 CONTINUE
      IF (T.LT.TSRT.OR.T.GT.TSRT+DTIM) GO TO 30
      DO 15 K=1,2
      J=INOX(K)
      IF (SPECIS(J).NE.ISPN(1)) GO TO 15
      XT(J)=DILUT*(XNAL-X(J))
      GO TO 20
   15 CONTINUE
      IF(NHC.EQ.0) GO TO 26
   20 DO 25 K=1,NHC
      J=IH(K)
      XT(J)=DILUT*(FALHC(K)*HCAL/CARB(K)-X(J))
   25 CONTINUE
   26 CONTINUE
      IF(NALD.EQ.0) GO TO 33
      DO 32 K=1,NALD
      J=IALD(K)
      XT(J)=DILUT*(FALALD(K)*HCAL/ALDCRB(K)-X(J))
   32 CONTINUE
   33 CONTINUE
   30 IF (T.GE.ESTOP) GO TO 65
      FNOW=Z1/HT
      I=IFIX(T/60.)
      ENOW=0.
      TT=(T-(I*60.))/60.
      I=(I+1)*5
      IF (NEM.GT.0) ENOW=((((TT*EC(I)+EC(I-1))*TT+EC(I-2))*TT+
     1EC(I-3))*TT+EC(I-4))/60.
      ENOW1=ENOW
      ENOW2=ENOW
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) ENOW1=((((TT*EH(I)+EH(I-1))*
     1TT+EH(I-2))*TT+EH(I-3))*TT+EH(I-4))/60.
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) ENOW2=((((TT*EX(I)+EX(I-1))
     1*TT+EX(I-2))*TT+EX(I-3))*TT+EX(I-4))/60.
      IF(ENOW1.LT.0.0) ENOW1=0.0
      IF(ENOW2.LT.0.0) ENOW2=0.0
      DO 45 K=1,2
      J=INOX(K)
      XT(J)=XT(J)+ENOW2*FNOW*EXN*FENX(K)
   45 CONTINUE
      IF (NALD.EQ.0) GO TO 55
      DO 50 K=1,NALD
      J=IALD(K)
      XT(J)=XT(J)+ENOW1*FNOW*EHC*ALDX(K)/ALDCRB(K)
   50 CONTINUE
   55 CONTINUE
      IF(NHC.EQ.0) GO TO 62
      DO 60 K=1,NHC
      J=IH(K)
      XT(J)=XT(J)+ENOW1*FNOW*EHC*RCTY(K)/CARB(K)
   60 CONTINUE
   62 CONTINUE
   65 IF (T.EQ.TOLD) GO TO 85
      IF (IP.EQ.0) GO TO 85
      I=IFIX(T/60.)
      I=I+2
      IF (I.GT.16) I=16
      Z=T/60.-FLOAT(I-2)
      II=0
      DO 80 JK=1,IP
      IR=IPH(JK)
      IK=KR(IR,1)
      DO 75 LK=1,8
      IF (SPECIS(IK).NE.PSPEC(LK)) GO TO 75
      J=II+LK
C     IF (P(I-1,J).EQ.0.) R(IR)=0.
C     IF (P(I-1,J).EQ.0.) GO TO 70
      R(IR)=((Z*CF(3*I-3,J)+CF(3*I-4,J))*Z+CF(3*I-5,J))*Z+P(I-1,J)
      R(IR)=R(IR)*RFCT(JK)
   70 II=0
      IF(LK.EQ.1) RK1=R(IR)
      IF (J.EQ.3.OR.J.EQ.5) II=1
      GO TO 80
   75 CONTINUE
   80 IF (R(IR).LT.0.) R(IR)=0.
      IF(KFACT.LE.0) GO TO 84
      DO 83 KP=1,KFACT
      DO 82 JK=1,IP
      IF(KPH(KP).NE.IPH(JK)) GO TO 82
      KNM=KPH(KP)
      R(KNM)=RFCT(JK)*RK1
      GO TO 83
   82 CONTINUE
   83 CONTINUE
   84 CONTINUE
   85 DO 110 IR=1,NR
      I=KR(IR,1)
      IF (I.EQ.0) GO TO 110
      IF (ITYPE(IR).EQ.2) GO TO 90
      IF (ITYPE(IR).EQ.3) GO TO 95
      IF (I.EQ.99) GO TO 101
      RT=R(IR)*X(I)
      GO TO 100
   90 J=KR(IR,2)
      RT=R(IR)*X(I)*X(J)
      XT(J)=XT(J)-RT
      GO TO 100
   95 J=KR(IR,2)
      K=KR(IR,3)
      RT=R(IR)*X(I)*X(J)*X(K)
      XT(J)=XT(J)-RT
      XT(K)=XT(K)-RT
  100 XT(I)=XT(I)-RT
  101 IF (I.EQ.99) RT=R(IR)
      DO 105 K=4,7
      I=KR(IR,K)
      IF (I.EQ.0) GO TO 110
  105 XT(I)=XT(I)+RT
  110 CONTINUE
      TOLD=T
      RETURN
C     ENTRY DIFSET
      ENTRY DIFSET (L,T,X,XT)
      TOLD=T
      IF (IP.EQ.0) RETURN
      II=0
      DO 125 J=1,IP
      IR=IPH(J)
      I=KR(IR,1)
      DO 120 K=1,8
      IF (SPECIS(I).NE.PSPEC(K)) GO TO 120
      R(IR)=P(1,K)*RFCT(J)
      IF(K.EQ.1) RK1=R(IR)
      IF (II.NE.1) GO TO 115
      R(IR)=P(1,K+1)*RFCT(J)
      II=0
      GO TO 125
  115 IF (K.EQ.3.OR.K.EQ.5) II=1
      GO TO 125
  120 CONTINUE
  125 CONTINUE
      IF(KFACT.LE.0) GO TO 384
      DO 383 KP=1,KFACT
      DO 382 JK=1,IP
      IF(KPH(KP).NE.IPH(JK)) GO TO 382
      KNM=KPH(KP)
      R(KNM)=RFCT(JK)*RK1
      GO TO 383
  382 CONTINUE
  383 CONTINUE
  384 CONTINUE
      RETURN
      END
```

SUBROUTINE OZMX

```
      SUBROUTINE OZMX (C,TL,TOUT,N0)
      DIMENSION C(N0,6), RUN(61), OZ(61)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FEX(2),CR(81),REACT(81),NI,PLSP
      NQ=JSTART
      IF (T.NE.START) GO TO 5
      RUN(1)=C(KOZ,1)
      NT=1
      TL=START+1.
      OZM=0.
      OZA=0.
      RETURN
    5 DO 10 I=1,61
      RR=(TL+FLOAT(I-1)-T)/H
      IF (RR.GT.0.) GO TO 15
      IF (TL+FLOAT(I-1).GT.STOPP) GO TO 15
      OZ(I)=C(KOZ,1)
      RH=1.
      DO 10 J=1,NQ
      RH=RH*RR
   10 OZ(I)=OZ(I)+RH*C(KOZ,J+1)
      I=61
   15 I=I-1
      TL=TL+FLOAT(I)
      DO 35 J=1,I
      IF (NT.GT.60) GO TO 25
      RUN(NT+1)=OZ(J)
      NT=NT+1
      IF (NT.LT.61) GO TO 35
      SIX=0.
      S2=RUN(60)
      DO 20 K=1,29
      SIX=SIX+RUN(2*K+1)
   20 S2=S2+RUN(2*K)
   25 OZA=2.*SIX+4.*S2+RUN(1)+OZ(J)
      SV=SIX
      SIX=S2-RUN(2)
      S2=SV+OZ(J)
      RUN(61)=OZ(J)
      DO 30 K=1,60
   30 RUN(K)=RUN(K+1)
      IF (OZA.GT.OZM) OZM=OZA
      IF (OZA.EQ.OZM) TM=TL+FLOAT(J-I-31)
   35 CONTINUE
      IF (TL-T.LT.0..AND.T.LT.STOPP) GO TO 5
      IF (NGO.NE.0) GO TO 40
      IF (T.GT.360..AND.OZA.LT.OZM) GO TO 45
   40 IF (T.LT.STOPP) RETURN
      GO TO 50
   45 TOUT=T
      STOPP=T
   50 OZM=OZM/180.
      OZA=OZA/180.
      IF (OZA.LT.OZM) RETURN
      IF (T.GT.STOPP.AND.OZM.GT.0.00001) TM=-TM
      RETURN
      END
```

SUBROUTINE COSET

```
      SUBROUTINE COSET (METH,NQ,EL,TQ,MAXDER)
      DIMENSION PERTST(12,2,3), EL(13), TQ(4)
      DATA PERTST/1.,1.,2.,1.,.3158,.07407,.01391,.002182,.0002945,.0000
     13492,.000003692,.0000003524,1.,1.,.5,.1667,.04167,1.,1.,1.,1.,1.,1
     2.,1.,2.,12.,24.,37.89,53.33,70.08,87.97,106.9,126.7,147.4,168.8,19
     31.0,2.0,4.5,7.333,10.42,13.7,1.,1.,1.,1.,1.,1.,1.,12.0,24.0,37.89,
     453.33,70.08,87.97,106.9,126.7,147.4,168.8,191.0,1.,3.0,6.0,9.167,1
     52.5,1.,1.,1.,1.,1.,1.,1.,1./
    5 MAXDER=5
      GO TO (10,15,20,25,30),NQ
   10 EL(1)=1.0
      GO TO 35
   15 EL(1)=6.6666666666667E-01
      EL(3)=3.3333333333333E-01
      GO TO 35
   20 EL(1)=5.4545454545455E-01
      EL(3)=EL(1)
      EL(4)=9.0909090909091E-02
      GO TO 35
   25 EL(1)=0.48
      EL(3)=0.7
      EL(4)=0.2
      EL(5)=0.02
      GO TO 35
   30 EL(1)=4.3795620437956E-01
      EL(3)=8.2116788321168E-01
      EL(4)=3.1021897810219E-01
      EL(5)=5.4744525547445E-02
      EL(6)=3.6496350364964E-03
   35 DO 40 K=1,3
   40 TQ(K)=PERTST(NQ,METH,K)
      TQ(4)=.5*TQ(2)/FLOAT(NQ+2)
      RETURN
      END
```

SUBROUTINE NSCORA

```
      SUBROUTINE NSCORA (N,IA,JA,A,IAP,AWORK,C,IR,ICT)
      INTEGER IA(1),JA(1),IAP(1),JAWORK(1500),C(1),IR(1),ICT(1)
      REAL A(1),AWORK(1)
      DO 5 K=1,N
      ICK=C(K)
    5 IR(ICK)=K
      JMIN=1
      DO 15 K=1,N
      ICK=C(K)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IF (JMIN.GT.JMAX) GO TO 15
      IAINK=IA(ICK)-1
      DO 10 J=JMIN,JMAX
      IAINK=IAINK+1
      JAOUTJ=JA(IAINK)
      JAOUTJ=IR(JAOUTJ)
      JAWORK(J)=JAOUTJ
   10 AWORK(J)=A(IAINK)
   15 JMIN=JMAX+1
      DO 20 I=1,N
   20 ICT(I)=IAP(I)
      JMIN=1
      DO 30 I=1,N
      ICK=C(I)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IF (JMIN.GT.JMAX) GO TO 30
      DO 25 J=JMIN,JMAX
      JAOUTJ=JAWORK(J)
      ICTJ=ICT(JAOUTJ)
      A(ICTJ)=AWORK(J)
      ICT(JAOUTJ)=ICTJ+1
   25 CONTINUE
   30 JMIN=JMAX+1
      RETURN
      END
```

SUBROUTINE NSNFAC

```
      SUBROUTINE NSNFAC (N,IA,JA,A,IL,JL,ISL,L,D,IU,JU,ISU,U,X,IRL,JRL,I
     1ER)
      INTEGER IA(1),JA(1),IL(1),JL(1),ISL(1)
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1)
      REAL A(1),L(1),D(1),U(1),X(1)
      REAL LKI
      IER=0
      DO 5 K=1,N
      IRL(K)=IL(K)
    5 JRL(K)=0
      DO 90 K=1,N
      X(K)=0.
      I1=0
      IF (JRL(K).EQ.0) GO TO 15
      I=JRL(K)
   10 I2=JRL(I)
      JRL(I)=I1
      I1=I
      X(I)=0.
      I=I2
      IF (I.NE.0) GO TO 10
   15 JMIN=ISU(K)
      JMAX=JMIN+IU(K+1)-IU(K)-1
      IF (JMIN.GT.JMAX) GO TO 25
      DO 20 J=JMIN,JMAX
      JUJ=JU(J)
   20 X(JUJ)=0.
   25 JMIN=IA(K)
      JMAX=IA(K+1)-1
      DO 30 J=JMIN,JMAX
      JAJ=JA(J)
   30 X(JAJ)=A(J)
      I=I1
      IF (I.EQ.0) GO TO 50
   35 IRLI=IRL(I)
      LKI=-X(I)
      L(IRLI)=-LKI
      JMIN=IU(I)
      JMAX=IU(I+1)-1
      IF (JMIN.GT.JMAX) GO TO 45
      ISUB=ISU(I)-1
      DO 40 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   40 X(JUJ)=X(JUJ)+LKI*U(J)
   45 I=JRL(I)
      IF (I.NE.0) GO TO 35
   50 IF (X(K).EQ.0.) GO TO 95
      DK=1./X(K)
      D(K)=DK
      IF (K.EQ.N) GO TO 90
      JMIN=IU(K)
      JMAX=IU(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 60
      ISUB=ISU(K)-1
      DO 55 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   55 U(J)=X(JUJ)*DK
   60 CONTINUE
      I=I1
      IF (I.EQ.0) GO TO 85
   65 IRL(I)=IRL(I)+1
      I1=JRL(I)
      IF (IRL(I).GE.IL(I+1)) GO TO 80
      ISLB=IRL(I)-IL(I)+ISL(I)
      J=JL(ISLB)
   70 IF (I.GT.JRL(J)) GO TO 75
      J=JRL(J)
      GO TO 70
```

```
75 JRL(I)=JRL(J)
   JRL(J)=I
80 I=I1
   IF (I.NE.0) GO TO 65
85 ISLK=ISL(K)
   IF (IRL(K).GE.IL(K+1)) GO TO 90
   J=JL(ISLK)
   JRL(K)=JRL(J)
   JRL(J)=K
90 CONTINUE
   RETURN
95 IER=K
   RETURN
   END
```

SUBROUTINE NSBSLV

```
      SUBROUTINE NSBSLV (N,R,C,IL,JL,ISL,L,D,IU,JU,ISU,U,X,B,Y)
      DIMENSION R(1), IL(1), JL(1), IU(1), JU(1), C(1), ISL(1), ISU(1)
      DIMENSION L(1), X(1), B(1), U(1), Y(1), D(1)
      INTEGER R,RK,C,CK
      REAL L
      DO 5 K=1,N
      RK=R(K)
    5 Y(K)=B(RK)
      DO 15 K=1,N
      JMIN=IL(K)
      JMAX=IL(K+1)-1
      YK=-D(K)*Y(K)
      Y(K)=-YK
      IF (JMIN.GT.JMAX) GO TO 15
      ISLB=ISL(K)-1
      DO 10 J=JMIN,JMAX
      ISLB=ISLB+1
      JLJ=JL(ISLB)
   10 Y(JLJ)=Y(JLJ)+YK*L(J)
   15 CONTINUE
      K=N
      DO 30 I=1,N
      SUM=-Y(K)
      JMIN=IU(K)
      JMAX=IU(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 25
      ISUB=ISU(K)-1
      DO 20 J=JMIN,JMAX
      ISUB=ISUB+1
      JUJ=JU(ISUB)
   20 SUM=SUM+U(J)*Y(JUJ)
   25 Y(K)=-SUM
      CK=C(K)
      X(CK)=-SUM
   30 K=K-1
      RETURN
      END
```

SUBROUTINE YSMER

```
      SUBROUTINE YSMER (A,K,A1)
      INTEGER A,A1(2)
      COMMON /INOUT/ INP,LOUT,ITAPE
      WRITE (LOUT,5) A,K,A1(1),A1(2)
    5 FORMAT (1X,A10,I6,2A10)
      RETURN
      END
```

SUBROUTINE INTERP

```
      SUBROUTINE INTERP (TOUT,Y,N0,Y0)
      COMMON /GEAR1/ T,H,DUMMY(4),N,IDUMMY(2),JSTART
      DIMENSION Y0(N0), Y(N0,1)
      DO 5 I=1,N
    5 Y0(I)=Y(I,1)
      L=JSTART+1
      S=(TOUT-T)/H
      S1=1.
      DO 15 J=2,L
      S1=S1*S
      DO 10 I=1,N
   10 Y0(I)=Y0(I)+S1*Y(I,J)
   15 CONTINUE
      RETURN
      END
```

SUBROUTINE LINER

```
      SUBROUTINE LINER (SIG,KALCMP,F)
      COMMON /NEED/ HC,XN,NL,NR,R(20),OZP(20),OZN(8,20),RHO(8,20),MR,OC(
     14),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      COMMON /VVLBL/ FACTR,DISTNC,CHRSZ,NCHR,OZLBL
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HCC,XNC,T
     1ICZ,DIGZ,CHRZ
      COMMON /CNTRL/ SGG,SIGMA,INFO,NPTO,TSTRT,DTIM,Z1,Z2,DCON,EHC,EXN,F
     1LST,TLST,NSPARS
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /TITL/ ITTL(18)
      COMMON /GEAR6/ RPL(20,20),RTL(20,20),NRL(20),NSL(20),NTL(20),NUL(2
     10),W(20),WW(20),OE(20),HCTP(20),XNE(20),XNEP(20),YP(20),TM(20),XNA
     2P(20),HCAP(20),HCLP(20),ITTL1(18),U(44),V(44),HCBP(20),DUM1(274)
      COMMON /MULPLT/HCSS,XNSS
      DIMENSION F(20), RBL(20,20), NBL(20), NTOL(20)
      DATA IBLANK/'    '/
C
C  FIRST SET CALCOMP OPTION
C
      CHRSZ=TICZ
      IDIG1=1
      IDIG2=2
      IHY=IFIX(HC*10.+0.5)
      IHZ=IFIX(XN*1000.+0.5)
      IF (MOD(IHY,10).NE.0) IDIG1=2
      IF (MOD(IHZ,7).NE.0.OR.IHZ.LT.10) IDIG2=3
      HCD=HCC/HC
      HCX=0.
      HCM=HC/10.
      XND=XNC/XN
      XNX=0.
      XNM=XN/7.
      XX=((10.0-(HCD*HC))/2.0)+0.3
      YY=((8.0-(XND*XN))/2.0)+0.3
      ORGY=-.75
      IF (KALCMP.LE.0) GO TO 5
      CALL PLOTS (I1,I2,14)
      CALL PLOT (XX,YY,-3)
    5 M=MR+1
      NLL=0
      NBLP=0
      DO 10 I=1,NL
      NUL(I)=0
      NTL(I)=0
      NTOL(I)=0
      NBL(I)=0
      NSL(I)=0
   10 NRL(I)=0
      DO 11 I=1,20
      DO 11 J=1,20
   11 RPL(I,J)=-9.
      OE(1)=OC(4)
      OE(2)=OS(2)
      XNE(1)=0.
      XNE(2)=XNS
      DO 15 I=1,NR
      K=NR+1-I
      OE(I+2)=OZN(MR,K)
      XNE(I+2)=HC/R(K)
      IF (XNE(I+2).GT.XN) GO TO 20
   15 CONTINUE
      I=NR+1
   20 I=I-1
      NE=I+2
      TOL=1.0-(0.17/(SQRT(FLOAT(NR))))
      NCR=(NR+1)/2
      CALL EDGMX (XNE,OE,NE,XMX,OZX,LX)
      NDIF=NE-LX+1
      NEW=NE
      NE=LX+1
      OE(NE)=OZX
      XNE(NE)=XMX
      CALL EDGMX (HCT,OT,NT,HMX,OZHX,LHX)
      NDIF1=NT-LHX+1
      NDIF2=NT-LHX-1
      NEW1=NT
      NT=LHX+1
      OT(NT)=OZHX
      HCT(NT)=HMX
      SX=-SIG*0.25
      IF (OZP(NL).LT.OC(2)) GO TO 25
      CALL NEWLIN (NT,OT,HCT,SX,LS,NL,1,0,HCTP,NPL,TOL,0,0,0)
      NTT=NPL
      IF (OZP(LS).GE.OC(2)) NLL=0
      IF (OZP(LS).GE.OC(2)) GO TO 45
   25 SX=-SIG*10.
      IF (NR.GT.1) GO TO 30
      OT(1)=OC(1)
      HCT(1)=0.
      OT(2)=OC(2)
      HCT(2)=XN
      MR2=2
      GO TO 40
   30 DO 35 II=1,MR
      OT(II+1)=OZN(II,1)
   35 HCT(II+1)=HCLL(II)
      OT(1)=OC(1)
      HCT(1)=0.
      MR2=MR+1
   40 CALL NEWLIN (MR2,OT,HCT,SX,LS,NL,2,0,HCLP,NLL,TOL,0,0,0)
      IF (OZP(NL).LT.OC(2)) NPL=NLL
   45 NPLI=NPL+1
      IF (NPLI.GE.NL) GO TO 55
      DO 50 J=NPLI,NL
   50 IF (OZP(J).LT.OE(NE)) NPL=NPL+1
   55 SX=-SIG*10.
      CALL NEWLIN (NE,OE,XNE,SX,LS,NL,3,0,XNEP,NEL,TOL,0,0,0)
      IF (OZP(LS).GE.OC(4)) GO TO 54
      SX=-SIG*10.
      IF (NR.GT.1) GO TO 51
      OE(1)=OC(1)
      XNE(1)=0.
      OE(2)=OC(2)
      XNE(2)=HC
      MR2=2
      GO TO 53
   51 DO 52 II=1,MR
      OE(II+1)=OZN(II,NR)
   52 XNE(II+1)=XNLL(II)
      OE(1)=OC(1)
      XNE(1)=0.
      MR2=MR+1
   53 CALL NEWLIN (MR2,OE,XNE,SX,LS,NL,2,0,HCBP,NBLP,TOL,0,0,0)
   54 CONTINUE
      IF (NDIF2.EQ.0) GO TO 70
      DO 60 II=LHX,NEW1
      JJ=LHX-II+1
      IF (IABS(JJ).GT.NCR) GO TO 65
      JO=II-LHX+1
      OT(JO)=OZN(MR,NCR+JJ-1)
   60 HCT(JO)=R(NCR+JJ-1)*XN
   65 OT(NDIF1)=OZHX
      HCT(NDIF1)=HMX
      SX=-SIG*10.
      CALL NEWLIN (NDIF1,OT,HCT,SX,NEL+1,NPL,4,NEL,HCAP,II,TOL,0,0,0)
   70 IF ((NTT+NLL).GE.NPL) GO TO 85
      DO 75 II=LX,NEW
      JJ=II-LX+1
      IF (JJ.GT.NCR) GO TO 80
      OE(JJ)=OZN(MR,NCR+JJ-1)
   75 XNE(JJ)=HC/R(NCR+JJ-1)
   80 OE(NDIF)=OZX
      XNE(NDIF)=XMX
      SX=-SIG*10.
      CALL NEWLIN (NDIF,OE,XNE,SX,NTT+1,NPL,5,NTT,XNAP,II,TOL,0,0,0)
   85 NR1=NR
      IF (OZP(LS).LT.OC(2).OR.OZP(LS).LT.OC(4)) NR1=NR-1
      NOZLST=0
      IF (OZP(LS).LT.OC(2)) IK=1
      IF (OZP(LS).GE.OC(2)) IK=0
      XOZ=AMAX1(OZHX,OZX,OC(3))
      IF (XOZ.EQ.OZHX) NOZLST=NT-2
      IF (XOZ.EQ.OC(3)) NOZLST=NCR
      IF (XOZ.EQ.OZX) NOZLST=NCR+NDIF-2
      DO 105 LL=1,NR1
      IF (OZP(LS).LT.OC(2)) I=LL+1
      IF (OZP(LS).GE.OC(2)) I=LL
      IF (NR.EQ.1) I=LL
      U(1)=OC(1)
      V(1)=0.
      DO 90 J=2,M
      U(J)=OZN(J-1,I)
   90 V(J)=RHO(J-1,I)
      SX=-SIG*3.0
      IF (M.GT.2) SX=-SIG*60./(FLOAT(M-2)**2)
      CALL EDGMX (V,U,M,HHMX,OZMMX,MM1)
      MM=MM1+1
      IF (MM.GE.M) GO TO 100
      U(MM)=OZMMX
      V(MM)=HHMX
      MDIF=M-MM1
      DO 95 J=1,MDIF
      W(J)=OZN(M-J,I)
   95 WW(J)=RHO(M-J,I)
      W(MDIF+1)=OZMMX
      WW(MDIF+1)=HHMX
      MDIF=MDIF+1
      IF ((LL-IK).LE.NOZLST) CALL NEWLIN (MDIF,W,WW,SX,LS,NL,6,0,RTL(1,I
     1),IJ,TOL,NUL,NTL,I)
      IF ((LL-IK).GT.NOZLST) CALL NEWLIN (MDIF,W,WW,SX,LS,NL,6,0,RBL(1,I
     1),IJ,TOL,NTOL,NBL,I)
      SX=-SIG*3.0
      IF (MM.GT.2) SX=-SIG*60./(FLOAT(MM-2)**2)
  100 CALL NEWLIN (MM,U,V,SX,LS,NL,7,0,RPL(1,I),II,TOL,NRL,NSL,I)
  105 CONTINUE
      CALL ISOPLT (HCTP,XN)
      SX=SIGMA*30./FLOAT(NR)
      NTT2=NTT+NLL
      IF (NTT.NE.0.AND.NLL.NE.0) NTT2=NTT
      NW=0
      DO 175 I=LS,NPL
      K=1
      IF (I.LE.NTT2) GO TO 110
      U(1)=HC
      V(1)=XNAP(I-NTT)
      GO TO 120
  110 IF (OZP(LS).GT.OC(2)) GO TO 115
      IF (I.GT.NLL) GO TO 115
      U(1)=0.
      V(1)=HCLP(I)
      GO TO 120
  115 U(1)=HCTP(I)
      V(1)=XN
  120 NT=NUL(I)
      NE=NTL(I)
      IF (NE.EQ.0) GO TO 130
      DO 125 JI=NE,NT
      J=NT-JI+1
      K=K+1
      V(K)=RTL(I,J)/F(J)
  125 U(K)=V(K)*R(J)
  130 NT=NRL(I)
      NE=NSL(I)
      IF (NE.EQ.0) GO TO 140
      DO 135 J=NE,NT
      K=K+1
      V(K)=RPL(I,J)/F(J)
  135 U(K)=V(K)*R(J)
  140 NT=NTOL(I)
      NE=NBL(I)
      IF (NE.EQ.0) GO TO 150
      DO 145 JI=NE,NT
      J=NT-JI+1
      K=K+1
      V(K)=RBL(I,J)/F(J)
  145 U(K)=V(K)*R(J)
  150 IF (OZP(LS).GT.OC(4)) GO TO 151
      IF (I.GT.NBLP) GO TO 151
      K=K+1
      U(K)=HCBP(I)
      V(K)=0.
      GO TO 160
  151 IF (I.GT.NEL) GO TO 155
      K=K+1
      U(K)=HC
      V(K)=XNEP(I)
      GO TO 160
  155 IF (NDIF2.EQ.0) GO TO 160
      K=K+1
      U(K)=HCAP(I-NEL)
      V(K)=XN
  160 U(K+1)=0.
      U(K+2)=1./HCD
      V(K+1)=0.
      V(K+2)=1./XND
      IF (K.LE.2) GO TO 175
      OZLBL=OZP(I)
      NW=NW+1
      W(NW)=OZP(I)
      NCHR=4
      NCNT=0
  165 VAL=OZLBL*(10.**NCNT)
      IF (VAL.GT.0.01) GO TO 170
      NCNT=NCNT+1
      GO TO 165
  170 NCHR=NCHR+NCNT
      REMB=OZLBL-FLOAT(IFIX(OZLBL*(10.**(NCNT+2))+0.1))/(10.**(NCNT+2))
      IF (REMB.GE.(0.001/(10.**NCNT))) NCHR=NCHR+1
      DO 171 IJ=1,K
      IF (U(IJ).GE.0..AND.V(IJ).GE.0.) GO TO 171
      NE=NSL(I)
      KN=NE+IJ-2
      XNE(1)=OC(1)
      WW(1)=0.
      DO 172 JJ=2,M
      XNE(JJ)=OZN(JJ-1,KN)
  172 WW(JJ)=RHO(JJ-1,KN)
      SSX=-50.
      IT=1
      CALL CURV1 (M,XNE,WW,SP1,SP2,YP,TM,SSX)
      U(IJ)=CURV2 (OZP(I),M,XNE,WW,YP,SSX,IT)
      V(IJ)=U(IJ)/F(KN)
      U(IJ)=V(IJ)*R(KN)
  171 CONTINUE
      CALL CURVE (U,V,K,1,KALCMP,0,0,SX)
  175 CONTINUE
      IF (KALCMP.LE.0) GO TO 210
      CALL FRAME (0.,0.,0.,HC,HCD,HCX,HCM,IDIG1,0.,XN,XND,XNX,XNM,IDIG2,
     19HNMHC,PPMC,9,7HNOX,PPM,7,1H ,1,1H ,1)
      NCNT=0
      DO 180 I=1,18
      IF (ITTL(I).NE.IBLANK) GO TO 185
      NCNT=NCNT+1
  180 CONTINUE
  185 NLST=18-NCNT
      DO 190 I=1,NLST
  190 ITTL1(I)=ITTL(I+NCNT)
      NCNT1=18
      DO 195 I=1,18
      II=19-I
      IF (ITTL1(II).NE.IBLANK) GO TO 200
      NCNT1=NCNT1-1
  195 CONTINUE
  200 NCNT1=NCNT1-NCNT
      ORGX=((HCD*HC)-(FLOAT(NCNT1)*4.*CHRZ))/2.0
      DO 205 I=1,NCNT1
      CALL SYMBOL (ORGX,ORGY,CHRZ,ITTL1(I),0.,4)
      ORGX=ORGX+4.0*CHRZ
  205 CONTINUE
      CALL PLOT (10.,2.,999)
  210 HCSS=FLOAT(NW)
      XNSS=FLOAT(NLL)
      CALL LINPRT (HC,XN)
      RETURN
      END
```

SUBROUTINE CURVE

```
      SUBROUTINE CURVE (XARRAY,YARRAY,NPTS,INC,KALCMP,LINTYP,INTEQ,SIGMA
     1)
C
C      *** PURPOSE -- PLOTS A SMOOTH CURVE THROUGH THE DATA VALUES FROM T
C          GW LUNDBERG,SAI   JULY  77
C
C           MODIFIED BY H HOGO AUG 1977
C
C         XARRAY  ARRAY CONTAINING X VALUES
C         YARRAY  ARRAY CONTIANING Y VALUES
C         NPTS    NUMBER OF DATA POINTS IN THE ARRAYS ACTUALLY USED
C                 ) 0  SCALING AT TOP OF ARRAYS
C         INC     EVERY INC POINT WILL BE USED
C         LINTYP  PLOT SPECIAL SYMBOL EVERY LINTYP POINT
C                 ) 0  CONNECTED SYMBOL PLOT
C                 = 0  LINE PLOT
C                 ( 0  UNCONNECTED SYMBOL PLOT
C         INTEQ   INTEGER EQUIVALENT OF SPECIAL SYMBOL
C         THIS ROUTINE CALLS  SYMBOL, PLOT, KURV1 AND KURV2
C
      COMMON /VVLBL/ FCTR,DIST,CHRSZ,NCHR,OZLBL
      COMMON /HOUR/ OZR,NGG,TM
      COMMON /NEED/ HC,XN,NL,NR,R(20),OZP(20),OZN(8,20),RHO(8,20),MR,OC(
     14),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      DIMENSION XARRAY(1), YARRAY(1), XI(50), YI(50), XP(50), YP(50), TE
     1MP(50)
C
      DATA NSLOPE/0/,SLOPE1,SLOPEN/0.,0./
C
C
C      *** LOCATE SCALING (FIRSTV AND DELTAV) FOR EACH ARRAY
C          ------ ------- ------- --- ------- --- ---- -----
C
C
C      *** SCALING IN TOP OF ARRAYS -- CALCOMP STANDARD
      N=NPTS*INC+1
      FIRSTX=XARRAY(N)
      FIRSTY=YARRAY(N)
      N=N+INC
      DELTAX=XARRAY(N)
      DELTAY=YARRAY(N)
C
      NUM=IABS(NPTS)
      IF (KALCMP.LE.0) GO TO 10
C
C      *** CHECK IF SYMBOL PLOT WANTED -- LINTYP () 0
      IF (LINTYP.EQ.0) GO TO 10
C
C      *** CENTERED SYMBOL PLOT
C          -------- ------ ----
C
C      *** SCALE FIRST DATA POINT AND PLOT CENTERED SYMBOL
      X=(XARRAY(1)-FIRSTX)/DELTAX
      Y=(YARRAY(1)-FIRSTY)/DELTAY
      CALL SYMBOL (X,Y,0.1,INTEQ,0.,-1)
C
C      *** PLOT REMAINING SYMBOLS AT INCREMENTS OF MARK
      MARK=IABS(LINTYP)
      N=1
C
      DO 5 J=2,NUM
      N=N+INC
      IF (MOD(N,MARK).NE.0) GO TO 5
      X=(XARRAY(N)-FIRSTX)/DELTAX
      Y=(YARRAY(N)-FIRSTY)/DELTAY
      CALL SYMBOL (X,Y,0.1,INTEQ,0.,-1)
    5 CONTINUE
C
C      *** IF THE SYMBOLS ARE NOT TO BE CONNECTED, RETURN
      IF (LINTYP.LT.0) GO TO 30
```

```
C
C     *** LINE PLOT (OR CONNECT SYMBOLS)
C         ---- ---- -- ------- --------
C
C     *** SCALE FIRST DATA POINT AND MOVE PEN THERE
   10 XI(1)=(XARRAY(1)-FIRSTX)/DELTAX
      YI(1)=(YARRAY(1)-FIRSTY)/DELTAY
C
C
C     *** SCALE THE REMAINING POINTS
      N=1
      DO 15 J=2,NUM
      N=N+INC
      XI(J)=(XARRAY(N)-FIRSTX)/DELTAX
      YI(J)=(YARRAY(N)-FIRSTY)/DELTAY
   15 CONTINUE
C
      NSLP=NSLOPE
C
C     *** CHECK IF PERIODIC
      IF (ABS(XI(NUM)-XI(1)).LT.0.01.AND.ABS(YI(NUM)-YI(1)).LT.0.01) NSL
     1P=-1
C
C     *** SET UP SPLINE INTERPOLATION
      NSLP=1
      SLOPE1=57.29578*ATAN((YI(1)-YI(2))/(XI(1)-XI(2)))
      IF (SLOPE1.GT.0.) SLOPE1=SLOPE1-180.
      SLOPE1=AMIN1(SLOPE1,-90.)
      SLOPEN=28.64789*ATAN((YI(N)-YI(N-1))/(XI(N)-XI(N-1)))
      CALL KURV1 (NUM,XI,YI,NSLP,SLOPE1,SLOPEN,XP,YP,TEMP,S,SIGMA)
      CALL KURV2 (0.,X,Y,NUM,XI,YI,XP,YP,S,SIGMA)
      X=AMAX1(0.,X)
      Y=AMAX1(0.,Y)
      USX=X*DELTAX+FIRSTX
      USY=Y*DELTAY+FIRSTY
      TM=1.
      CALL SAVLIN (USX,USY)
      TM=2.
C
C     *** LINE SEGMENTS WILL BE A TENTH INCH LONG -- S IS THE ARCLENGTH
      NP=10.*S+1
      CONST=1./NP
      DIST=S
      IF (KALCMP.LE.0) GO TO 20
      IF (USX.GT.HC.OR.USY.GT.XN) GO TO 20
      CALL VVLBLF (XI(1),YI(1))
C
C     *** MAP AND PLOT SEGMENTS
   20 DO 25 J=1,NP
      T=-J*CONST
      CALL KURV2 (T,X,Y,NUM,XI,YI,XP,YP,S,SIGMA)
      X=AMAX1(0.,X)
      Y=AMAX1(0.,Y)
      USX=X*DELTAX+FIRSTX
      USY=Y*DELTAY+FIRSTY
      CALL SAVLIN (USX,USY)
      IF (KALCMP.LE.0) GO TO 25
      IF (USX.GT.HC.OR.USY.GT.XN) GO TO 25
      CALL VVLBLC (X,Y)
   25 CONTINUE
      IF (KALCMP.LE.0) GO TO 30
      IF (USX.GT.HC.OR.USY.GT.XN) GO TO 30
      CALL VVLBLL (0.,0.)
C
   30 RETURN
C
      END
```

SUBROUTINE ISOPLT

```
      SUBROUTINE ISOPLT (SAVHC,SAVNOX)
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZZ(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      COMMON /TITL/ ITTL(18)
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),ND,PLSP
      COMMON /GEAR6/ DUM1(880),OZP(20),DUM2(326),NGRID(101,2),DUM3(72)
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /MULPLT/HCSS,XNSS
      DIMENSION TVERT(52,2), TPRINT(11), NLINE(3)
      DIMENSION CVERT(9), TV(7), SAVDAT(101), TV1(7)
      DIMENSION JGRID(101,42)
      INTEGER PLSP
      DATA JBLANK/4H    /,MAXHC/101/,MAXNOX/42/,TGRID/100./,
     1CGRID/42./,JPLUS/1H+/,JBAR/1HI/,JSYMB/1H+/
      DATA CVERT/4H O  ,4H Z  ,4H O  ,4H N  ,4H E  ,4H    ,4H P  ,4H P
     1,4H M  /
      DATA TV/4H N  ,4H O  ,4H X  ,4H    ,4H P  ,4H P  ,4H M  /
      DATA TVERT/104*4H    /
      DATA IBLANK/4H    /,BLANK/4H    /,IOCHAR/1HO/,IBLK/1H /
      NR1=1
      DO 5 J=1,42
      IF (J.LE.2) NGRID(1,J)=JBAR
      IF (J.LE.2) NGRID(101,J)=JBAR
      JGRID(1,J)=JBAR
      JGRID(101,J)=JBAR
    5 CONTINUE
      DO 15 I=1,52
      TVERT(I,1)=BLANK
      IF (NPTO.EQ.0) GO TO 10
      IF (I.LT.18.OR.I.GT.26) GO TO 15
      K=I-17
      TVERT(I,1)=CVERT(K)
      GO TO 15
   10 IF (I.LT.17.OR.I.GT.23) GO TO 15
      K=I-16
      TVERT(I,1)=TV(K)
   15 CONTINUE
      DO 20 I=1,101
   20 SAVDAT(I)=0.
      DO 25 J=1,42,3
      JGRID(1,J)=JPLUS
      JGRID(101,J)=JPLUS
   25 CONTINUE
C
C SET NORMALIZATION FACTORS AND VERTICAL LABELS
C
      CLOW=0.
      TLOW=0.
      IF (NPTO.NE.0) GO TO 35
      CHIGH=XN
      CSPAN=CGRID/CHIGH
      THIGH=HC
      DO 30 I=1,7
      M=8-I
      TV1(I)=(FLOAT(M)/7.)*CHIGH
   30 CONTINUE
      GO TO 40
C
C SET HORIZONTAL LABELS
C
   35 THIGH=STOPP
   40 TSPAN=TGRID/THIGH
      DO 45 J=1,11
      TPRINT(J)=(FLOAT(J-1)/10.)*THIGH
   45 CONTINUE
C
C CLEAR GRID
C
      MAXHC1=MAXHC-1
      DO 50 K=1,MAXNOX
      DO 50 J=2,MAXHC1
      JGRID(J,K)=JBLANK
      IF (K.LE.2) NGRID(J,K)=JBLANK
   50 CONTINUE
      RETURN
C
C ENTRY FOR SAVING INTERPOLATED POINTS
C
C     ENTRY SAVLIN
      ENTRY SAVLIN (SAVHC,SAVNOX)
      KHC=IFIX((SAVHC-TLOW)*TSPAN+1.5)
      IF (NPTO.NE.0) GO TO 55
      KNOX=IFIX((SAVNOX-CLOW)*CSPAN-0.5)
      KNOX=MAXNOX-KNOX
      IF (KNOX.LT.1) GO TO 60
      IF (KNOX.GT.MAXNOX) GO TO 60
   55 IF (KHC.LT.1) GO TO 60
      IF (KHC.GT.MAXHC1) GO TO 60
      IF (NPTO.EQ.0) JGRID(KHC,KNOX)=JSYMB
      IF (NPTO.NE.0) GO TO 56
      IF (TM.EQ.1..AND.NPTO.EQ.0) DUM3(NR1)=FLOAT(KHC)
      IF (TM.EQ.1.) NR1=NR1+1
      IF (KHC.LT.2) GO TO 60
   56 CONTINUE
      IF (NPTO.NE.0) SAVDAT(KHC)=SAVNOX
   60 RETURN
C
C ENTRY FOR PLOTTING GRID
C
C     ENTRY LINPRT
      ENTRY LINPRT (SAVHC,SAVNOX)
      IF (NPTO.NE.0) GO TO 95
      NPL=IFIX(HCSS+0.1)
      NLL=IFIX(XNSS+0.5)
      KOUNT=0
      IF (NLL.EQ.0) GO TO 80
      NJ=1
   65 NJ=NJ+1
      J=MAXNOX-NJ
      IF (JGRID(3,J).EQ.JBLANK) GO TO 65
      KOUNT=KOUNT+1
      IF (KOUNT.GT.NLL) GO TO 75
      IF (NJ.GT.MAXNOX-1) GO TO 75
      NVAR=IFIX(OZP(KOUNT)*100.+0.5)
      CALL CONVT (NVAR,NLINE)
      DO 70 II=1,3
      IF (NLINE(II).NE.IBLANK) JGRID(2+II,J)=NLINE(II)
   70 CONTINUE
      NJ=NJ+1
      GO TO 65
   75 KOUNT=KOUNT-1
   80 KOUNT=KOUNT+1
      NR1=NR1-1
      DO 90 I=KOUNT,NR1
      NVAR=IFIX(OZP(I)*100.+0.5)
      CALL CONVT (NVAR,NLINE)
      KHC=IFIX(DUM3(I)+0.1)
      DO 85 II=2,3
      IF (NLINE(II).NE.IBLK) NGRID(KHC,II-1)=NLINE(II)
   85 CONTINUE
   90 CONTINUE
      GO TO 110
   95 CHIGH=OZM+(0.2*OZM)
```

```
      IF (OZM.EQ.0.0) RETURN
      CSPAN=CGRID/CHIGH
      DO 100 I=1,7
      M=8-I
      TV1(I)=(FLOAT(M)/7.)*CHIGH
  100 CONTINUE
      DO 105 I=2,100
      IF (SAVDAT(I).EQ.0.) GO TO 105
      KNOX=IFIX(SAVDAT(I)*CSPAN-0.5)
      KNOX=MAXNOX-KNOX
      IF (KNOX.LT.1) GO TO 105
      IF (KNOX.GT.MAXNOX) GO TO 105
      JGRID(I,KNOX)=IOCHAR
  105 CONTINUE
  110 IF (NPTO.EQ.0) WRITE (IOUT,125) ((NGRID(I,J),I=1,101),J=1,2)
      IF (NPTO.NE.0) WRITE (IOUT,120) TVERT(1,1),TV1(1)
      IF (NPTO.EQ.0) KFRST=1
      IF (NPTO.NE.0) KFRST=2
      DO 115 K=KFRST,MAXNOX
      L=MOD((K-1),6)
      I=(K-1)/6+1
      IF (L.EQ.0) WRITE (IOUT,130) TVERT(K,1),TV1(I),(JGRID(J,K),J=1,MAX
     1HC)
      IF (L.NE.0) WRITE (IOUT,135) TVERT(K,1),(JGRID(J,K),J=1,MAXHC)
  115 CONTINUE
      WRITE (IOUT,140) CLOW
      IF (NPTO.EQ.0) WRITE (IOUT,145) TPRINT
      IF (NPTO.NE.0) WRITE (IOUT,155) TPRINT
      WRITE (IOUT,150) (ITTL(I),I=1,18)
      IF (NPTO.EQ.0) WRITE (IOUT,160) PLSP,(OZP(I),I=1,NPL)
      RETURN
C
C
  120 FORMAT (1H1,//////////,9X,A4,F5.3,1H+,10(10H---------+))
  125 FORMAT (1H1,//////,18X,1H+,10(10H---------+),/,18X,101A1,/,18X,101
     1A1)
  130 FORMAT (9X,A4,F5.3,101A1)
  135 FORMAT (9X,A4,5X,101A1)
  140 FORMAT (13X,F5.3,1H+,10(10H---------+))
  145 FORMAT (F21.3,10F10.2,/,64X,11HNMHC (PPMC),//)
  150 FORMAT (46X,18A4)
  155 FORMAT (F21.1,10F10.1,/,63X,14HTIME (MINUTES),//)
  160 FORMAT (1H0,/,20X,4HTHE ,A4,12H LINES ARE  ,10F8.5,/,40X,10F8.5)
      END
```

SUBROUTINE CURV1

```
      SUBROUTINE CURV1 (N,X,Y,SLP1,SLPN,YP,TEMP,SIGMA)
C
C    THIS SUBROUTINE DETERMINES THE PARAMETERS NECESSARY TO
C    COMPUTE AN INTERPOLATORY SPLINE UNDER TENSION THROUGH
C    A SEQUENCE OF FUNCTIONAL VALUES.  THE SLOPES AT THE TWO
C    ENDS OF THE CURVE MAY BE SPECIFIED OR OMITTED.  FOR ACTUAL
C    COMPUTATION OF POINTS ON THE CURVE IT IS NECESSARY TO CALL
C    THE FUNCTION CURV2.
C
C    ON INPUT --
C    N = THE NUMBER OF VALUES TO BE INTERPOLATED (N.GE.2),
C    X = AN ARRAY OF THE N INCREASING ABCISSAE OF THE
C        FUNCTIONAL VALUES,
C    Y = AN ARRAY OF THE N ORDINATES OF THE VALUES, (I.E.Y(K)
C        IS THE FUNCTIONAL VALUE CORRESPONDING TO X(K)),
C    SLP1,SLPN CONTAIN THE DESIRED VALUES FOR THE FIRST
C        DERIVATIVE TO THE CURVE AT X(1) AND X(N), RESPECTIVELY,
C        IF THE QUANTITY SIGMA IS NEGATIVE THESE VALUES WILL BE
C        DETERMINED INTERNALLY AND THE USER NEED ONLY FURNISH
C        PLACE-HOLDING PARAMETERS FOR SLP1 AND SLPN.  SUCH PLACE-
C        HOLDING PARAMETERS WILL BE IGNORED BY NOT DESTROYED,
C    YP = AN ARRAY OF LENGTH AT LEAST N
C    TEMP = AN ARRAY OF LENGTH AT LEAST N WHICH IS USED FOR
C        SCRATCH STORAGE,
C    SIGMA = THE TENSION FACTOR.  THIS IS NON-ZERO AND
C        INDICATES THE CURVINESS DESIRED. IF ABS(SIGMA) IS NEARLY
C        ZERO (E.G. .001) THE RESULTING CURVE IS APPROXIMATELY A
C        CUBIC SPLINE.  IF ABS(SIGMA) IS LARGE (E.G. 50.) THE
C        RESULTING CURVE IS NEARLY A POLYGONAL LINE.  THE SIGN
C        OF SIGMA INDICATES WHETHER THE DERIVATIVE INFORMATION
C        HAS BEEN INPUT OR NOT.  IF SIGMA IS NEGATIVE THE ENDPOINT
C        DERIVATIVES WILL BE DETERMINED INTERNALLY.  A STANDARD
C        VALUE FOR SIGMA IS APPROXIMATELY 1. IN ABSOLUTE VALUE
C
C    ON OUTPUT --
C    YP = VALUES PROPORTIONAL TO THE SECOND DERIVATIVE
C        OF THE CURVE AT THE GIVEN NODES.
C    N,X,Y,SLP1 AND SIGMA ARE UNALTERED,
C
C     *** AK CLINE/NCAR, COMM. ACM 17,4(APR.1974), 221.
C
      COMMON /MEXP/EXPMAX
      DIMENSION X(N), Y(N), YP(N), TEMP(N)
C
      NCYC=0
      NCHG=0
      NM1=N-1
      NP1=N+1
      DELX1=X(2)-X(1)
      IF (ABS(DELX1/X(2)).LT.0.02) GO TO 55
      DX1=(Y(2)-Y(1))/DELX1
C
C     *** DETERMINE SLOPES IF NECESSARY
      IF (SIGMA.LT.0.) GO TO 45
      SLPP1=SLP1
      SLPPN=SLPN
C
C     *** DENORMALIZE TENSION FACTOR
    5 IF (ABS(X(N)-X(1))/X(N).LT.0.02) GO TO 55
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/(X(N)-X(1))
      DX1=(Y(2)-Y(1))/DELX1
C
C     *** SET UP RIGHT HAND SIDE OF TRIDIAGONAL SYSTEM
C         FOR YP AND PERFORM FORWARD ELIMINATION
      DELS=SIGMAP*DELX1
      IF (DELS.GE.EXPMAX) GO TO 55
      EXPS=EXP(DELS)
      SINHS=0.5*(EXPS-1./EXPS)
      SINHIN=1./(DELX1*SINHS)
      DIAG1=SINHIN*(DELS*0.5*(EXPS+1./EXPS)-SINHS)
      DIAGIN=1./DIAG1
      YP(1)=DIAGIN*(DX1-SLPP1)
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(1)=DIAGIN*SPDIAG
      IF (N.EQ.2) GO TO 15
      DO 10 I=2,NM1
      DELX2=X(I+1)-X(I)
      IF (ABS(DELX2)/X(I+1).LT.0.02) GO TO 55
      DX2=(Y(I+1)-Y(I))/DELX2
      DELS=SIGMAP*DELX2
      IF (DELS.GE.EXPMAX) GO TO 55
      EXPS=EXP(DELS)
      SINHS=.5*(EXPS-1./EXPS)
      SINHIN=1./(DELX2*SINHS)
      DIAG2=SINHIN*(DELS*(.5*(EXPS+1./EXPS))-SINHS)
      DIAGIN=1./(DIAG1+DIAG2-SPDIAG*TEMP(I-1))
      YP(I)=DIAGIN*(DX2-DX1-SPDIAG*YP(I-1))
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(I)=DIAGIN*SPDIAG
      DX1=DX2
      DIAG1=DIAG2
   10 CONTINUE
   15 DIAGIN=1./(DIAG1-SPDIAG*TEMP(NM1))
      YP(N)=DIAGIN*(SLPPN-DX2-SPDIAG*YP(NM1))
C
C     ***  PERFORM BACK SUBSTITUTION
      DO 20 I=2,N
      IBAK=NP1-I
      YP(IBAK)=YP(IBAK)-TEMP(IBAK)*YP(IBAK+1)
   20 CONTINUE
      IF (SIGMA.GT.0.) RETURN
      IF (N.EQ.3) RETURN
      IF (NCYC.GT.15) RETURN
      IF (NCYC.GT.0) GO TO 25
      XTEST=(X(3)+X(2))/2.
      YCORD=(Y(3)+Y(2))/2.
      FACT=SQRT(ABS(SIGMA))
      YTEST=(YCORD*FACT+CIRC(XTEST,X(1),Y(1))+CIRC(XTEST,X(2),Y(2)))/(2.
     1+FACT)
      DY2=CURV2(XTEST,N,X,Y,YP,SIGMA,1)-YTEST
      DSAV=DY2
      SN=-1.
      IF (DY2.GT.0.) SN=1.
      FACT=0.3*(SN+2.)
      DY2=0.
      IT=1
   25 NCYC=NCYC+1
      DY1=DY2
      DY2=CURV2(XTEST,N,X,Y,YP,SIGMA,IT)-YTEST
      IF (NCYC.GT.15) RETURN
      IF (NCYC.GT.13.AND.NCHG.LT.2) GO TO 40
      IF (SIGN(1.,DY1).NE.SIGN(1.,DY2)) GO TO 30
      IF (ABS(DY2).LT.ABS(DY1)) GO TO 35
   30 SN=-SN
      NCHG=NCHG+1
      FACT=SN*((1./(1.-SN*FACT))**(1./3.)-1.)
   35 SLPP1=SLPP1*(1.+SN*FACT)
      GO TO 5
C
   40 IF (DY2/DSAV.LT.0.2) GO TO 35
      SLPP1=SLPPX
      NCYC=15
      GO TO 5
   45 IF (N.EQ.2) GO TO 50
C
C     *** IF NO DERIVATIVES ARE GIVEN USE SECOND ORDER POLYNOMIAL
C         INTERPOLATION ON INPUT DATA FOR VALUES AT ENDPOINTS.
      SLPP1=(Y(2)-Y(1))/(X(2)-X(1))
      DELN=X(N)-X(NM1)
      DELNM1=X(NM1)-X(N-2)
      DELNN=X(N)-X(N-2)
      IF (ABS(DELN)/X(N).LT.0.02) GO TO 55
      IF (ABS(DELN)/X(N).LT.0.02) GO TO 55
      IF (ABS(DELNM1)/X(NM1).LT.0.02) GO TO 55
      IF (ABS(DELNN)/X(N).LT.0.02) GO TO 55
      C1=(DELNN+DELN)/DELNN/DELN
      C2=-DELNN/DELN/DELNM1
      C3=DELN/DELNN/DELNM1
      SLPPN=C3*Y(N-2)+C2*Y(NM1)+C1*Y(N)
      DX2=X(3)-X(2)
      DX31=X(3)-X(1)
      IF (ABS(DX2)/X(3).LT.0.02) GO TO 55
      IF (ABS(DX31)/X(3).LT.0.02) GO TO 55
      C1=-(DX31+DELX1)/DX31/DELX1
      C2=DX31/DELX1/DX2
      C3=-DELX1/DX31/DX2
      SLPPX=C1*Y(1)+C2*Y(2)+C3*Y(3)
      IF (Y(2).GT.Y(1)) SLPPX=AMAX1(0.,SLPPX)
      FACT2=SQRT(ABS(SIGMA))
      SLPPX=(SLPPX+FACT2*SLPP1)/(1.+FACT2)
      SLPP1=SLPPX
      IF (Y(N).GT.Y(NM1)) SLPPN=AMAX1(0.,SLPPN)
      SLPNL=(Y(N)-Y(NM1))/DELN
      SLPPN=(SLPPN+SLPNL*FACT2)/(1.+FACT2)
      SLPPN=(SLPPN-SLPNL*SIGMA)/(1.-SIGMA)
      GO TO 5
C
C     *** IF ONLY TWO POINTS AND NO DERIVATIVES ARE GIVEN, USE
C         STRAIGHT LINE FOR CURVE
C
   50 YP(1)=0.
      YP(2)=0.
      RETURN
   55 SIGMA=-50.
      RETURN
      END
```

FUNCTION CURV2

```
      FUNCTION CURV2 (T,N,X,Y,YP,SIGMA,IT)
C
C    THIS FUNCTION INTERPOLATES A CURVE AT A GIVEN POINT
C    USING A SPLINE UNDER TENSION.  THE SUBROUTINE CURV1 SHOULD
C    BE CALLED EARLIER TO DETERMINE CERTAIN NECESSARY
C    PARAMETERS.
C
C    ON INPUT--
C    T = A REAL VALUE TO BE MAPPED ONTO THE
C        INTERPOLATING CURVE.
C    N = THE NUMBER OF POINTS WHICH WERE INTERPOLATED
C        TO DETERMINE THE CURVE,
C    X,Y = ARRAYS CONTAINING THE ORDINATES AND ABCISSAS
C        OF THE INTERPOLATED POINTS,
C    YP = AN ARRAY WITH VALUES PROPORTIONAL TO THE SECOND
C        DERIVATIVE OF THE CURVE AT THE NODES
C    SIGMA = THE TENSION FACTOR (ITS SIGN IS IGNORED)
C        IT IS AN INTEGER SWITCH.  IF IT IS NOT 1 THIS INDICATES
C        THAT THE FUNCTION HAS BEEN CALLED PREVIOUSLY (WITH N,X,
C        Y,YP, AND SIGMA UNALTERED) AND THAT THIS VALUE OF T
C        EXCEEDS THE PREVIOUS VALUE.  WITH SUCH INFORMATION THE
C        FUNCTION IS ABLE TO PERFORM THE INTERPOLATION MUCH MORE
C        RAPIDLY.  IF A USER SEEKS TO INTERPOLATE AT A SEQUENCE
C        OF POINTS, EFFICIENCY IS GAINED BY ORDERING THE VALUES
C        INCREASING AND SETTING IT TO THE INDEX OF THE CALL.
C        IF IT IS 1 THE SEARCH FOR THE INTERVAL (X(K),X(K+1))
C        CONTAINING T STARTS WITH K=1.
C        THE PARAMETERS N,X,Y,YP AND SIGMA SHOULD BE INPUT
C        UNALTERED FROM THE OUTPUT OF CURV1.
C
C    ON OUTPUT--
C    CURV2 = THE INTERPOLATED VALUE.  FOR T LESS THAN
C        X(1) CURV2 = Y(1).  FOR T GREATER THAN X(N) CURV2 = Y(N).
C
C    NONE OF THE INPUT PARAMETERS ARE ALTERED.
C
C     *** AK CLINE/NCAR, COMM. ACM 17,4(APR.1974), 221
C
      DIMENSION X(N), Y(N), YP(N)
C
      S=X(N)-X(1)
      IT=IABS(IT)
C
C     *** DENORMALIZE SIGMA
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S
C
C     *** IF IT.NE. 1 START SEARCH WHERE PREVIOUSLY TERMINATED,
C         OTHERWISE START SEARCH FROM BEGINNING
      IF (IT.EQ.1) I1=2
C
C     *** SEARCH FOR INTERVAL
    5 DO 10 I=I1,N
      IF (X(I)-T) 10,10,15
   10 CONTINUE
      I=N
C
C     *** CHECK TO INSURE CORRECT INTERVAL
   15 IF (X(I-1).LE.T.OR.T.LE.X(1)) GO TO 20
C
C     *** RESTART SEARCH AND RESET I1
C          (INPUT (IT( WAS INCORRECT)
      I1=2
      GO TO 5
C
C     *** SET UP AND PERFORM INTERPOLATION
   20 IF (SIGMA.EQ.-50.) GO TO 25
      DEL1=T-X(I-1)
      DEL2=X(I)-T
      DELS=X(I)-X(I-1)
      EXPS1=EXP(SIGMAP*DEL1)
      SINHD1=.5*(EXPS1-1./EXPS1)
      EXPS=EXP(SIGMAP*DEL2)
      SINHD2=.5*(EXPS-1./EXPS)
      EXPS=EXPS1*EXPS
      SINHS=.5*(EXPS-1./EXPS)
      CURV2=(YP(I)*SINHD1+YP(I-1)*SINHD2)/SINHS+((Y(I)-YP(I))*DEL1+(Y(I-
     11)-YP(I-1))*DEL2)/DELS
      IF ((ABS(Y(I)-CURV2)+ABS(Y(I-1)-CURV2)).GT.1.001*(ABS(Y(I)-Y(I-1))
     1)) IT=-IT
      I1=I
      RETURN
   25 IF (ABS(X(I)-X(I-1))/X(I).LT.0.02) I=I+1
      IF (I.GT.N) I=I-2
      CURV2=((T-X(I-1))*(Y(I)-Y(I-1))/(X(I)-X(I-1)))+Y(I-1)
      IT=1
      RETURN
      END
```

SUBROUTINE KURV1

```
      SUBROUTINE KURV1 (NPTS,X,Y,NSLOPE,SLOPE1,SLOPEN,XP,YP,TEMP,S,SIGMA
     1)
C
C     THIS SUBROUTINE DETERMINES THE PARAMETERS NECESSARY TO
C     COMPUTE AN SPLINE UNDER TENSION PASSING THROUGH A SEQUENCE
C     OF PAIRS (X(1),Y(1),....,X(N),Y(N)) IN THE PLANE, THE
C     SLOPES AT THE TWO ENDS OF THE CURVE MAY BE SPECIFIED OR
C     OMITTED, FOR ACTUAL COMPUTATION OF POINTS ON THE CURVE IT
C     IS NECESSARY TO CALL THE SUBROUTINE KURV2.
C
C     ON INPUT --
C     NPTS = THE NUMBER OF POINTS TO BE INTERPOLATED (N.GE.2),
C     X = AN ARRAY CONTAINING THE N X-COORDINATES OF THE
C         POINTS,
C     Y = AN ARRAY CONTAIING THE N Y-COODINATES OF THE
C         POINTS,
C     NSLOPE = A FLAG FOR ENDPOINT SLOPES.  IF \ 0, THIS IS A CLOSED
C         LOOP AND NO SLOPES ARE GIVEN.  IF = 0, THIS IS AN OPEN CURVE
C         AND NO SLOPES ARE GIVEN.  IF ) 0, BOTH ENDPOINT SLOPES ARE
C         GIVEN
C     SLOPE1,SLOPEN = THE DESIRED VALUES FOR THE SLOPE
C         OF THE CURVE AT (X(1),Y(1)) AND (X(N),Y(N)), RESPEC-
C         TIVELY.  THESE QUANTITIES ARE IN DEGREES AND MEASURED
C         COUNTER CLOCKWISE FROM THE POSITIVE X-AXIS.  THE POSITIVE
C         SENSE OF THE CURVE IS ASSUMED TO BE THAT MOVING FROM THE
C         POINT 1 TO POINT N.
C     XP,YP = ARRAYS OF LENGTH AT LEAST N,
C     TEMP = AN ARRAY OF LENGTH AT LEAST N WHICH IS USED FOR
C         SCRATCH STORAGE,
C     SIGMA = THE TENSION FACTOR.  THIS IS NON-ZERO AND
C         INDICATES THE CURVINESS DESIRED.  IF SIGMA IS VERY
C         LARGE (E.G. 50.) THE RESULTING CURVE IS VERY NEARLY A
C         POLYGONAL LINE.  A STANDARD VALUE FOR SIGMA IS 1.
C
C     ON OUTPUT -
C     N,X,Y,SLOPE1,SLOPEN, AND SIGMA ARE UNALTERED,
C     XP,YP CONTAIN INFORMATION ABOUT THE CURVATURE OF THE
C         CURVE AT THE GIVEN NODE,
C     S = THE POLYGONAL ARCLENGTH OF THE CURVE.
C
C      *** AK CLINE, COMM. ACM 17,4(APR.1974), 221
C          MODIFIED BY GW LUNDBERG/SAI  MAY !77
C
      DIMENSION X(NPTS), Y(NPTS), XP(NPTS), YP(NPTS), TEMP(NPTS)
C
      COMMON /MEXP/EXPMAX
      TEMAX=-9999.
      DEGRAD=3.1415926/180.
      N=NPTS
      SLP1=SLOPE1
      SLPN=SLOPEN
      NM1=N-1
      NP1=N+1
      DELX1=X(2)-X(1)
      DELY1=Y(2)-Y(1)
      DELS1=SQRT(DELX1*DELX1+DELY1*DELY1)
      DX1=DELX1/DELS1
      DY1=DELY1/DELS1
C
C      *** DETERMINE SLOPES IF NECESSARY
      IF (NSLOPE) 55,45,5
    5 SLPP1=SLP1*DEGRAD
      SLPPN=SLPN*DEGRAD
C
C     *** SET UP RIGHT HAND SIDES OF TRIDIAGONAL LINEAR SYSTEM FOR
C         XP AND YP
   10 XP(1)=DX1-COS(SLPP1)
      YP(1)=DY1-SIN(SLPP1)
      TEMP(1)=DELS1
      S=DELS1
      IF (N.EQ.2) GO TO 20
      DO 15 I=2,NM1
      DELX2=X(I+1)-X(I)
      DELY2=Y(I+1)-Y(I)
      DELS2=SQRT(DELX2*DELX2+DELY2*DELY2)
      DX2=DELX2/DELS2
      DY2=DELY2/DELS2
      XP(I)=DX2-DX1
      YP(I)=DY2-DY1
      TEMP(I)=DELS2
      TEMAX=AMAX1(TEMAX,TEMP(I))
      DELX1=DELX2
      DELY1=DELY2
      DELS1=DELS2
      DX1=DX2
      DY1=DY2
C
C     *** ACCUMULATE POLYGONAL ARCLENGTH
      S=S+DELS1
   15 CONTINUE
   20 XP(N)=COS(SLPPN)-DX1
      YP(N)=SIN(SLPPN)-DY1
C
C     *** DENORMALIZE TENSION FACTOR
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S
      DELT1=SIGMAP*TEMAX
      IF (DELT1.LT.EXPMAX) GO TO 25
      SIGMAP=0.9*EXPMAX/TEMAX
      SGN=1.0
      IF (SIGMA.LT.0.) SGN=-1.0
      SIGMA=SIGMAP*SGN*S/FLOAT(N-1)
   25 CONTINUE
C
C     *** PERFORM FORWARD ELIMINATION ON TRIDIAGONAL SYSTEM
      DELS=SIGMAP*TEMP(1)
      EXPS=EXP(DELS)
      SINHS=.5*(EXPS-1./EXPS)
      SINHIN=1./(TEMP(1)*SINHS)
      DIAG1=SINHIN*(DELS*.5*(EXPS+1./EXPS)-SINHS)
      DIAGIN=1./DIAG1
      XP(1)=DIAGIN*XP(1)
      YP(1)=DIAGIN*YP(1)
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(1)=DIAGIN*SPDIAG
      IF (N.EQ.2) GO TO 35
      DO 30 I=2,NM1
      DELS=SIGMAP*TEMP(I)
      EXPS=EXP(DELS)
      SINHS=.5*(EXPS-1./EXPS)
      SINHIN=1./(TEMP(I)*SINHS)
      DIAG2=SINHIN*(DELS*(.5*(EXPS+1./EXPS))-SINHS)
      DIAGIN=1./(DIAG1+DIAG2-SPDIAG*TEMP(I-1))
      XP(I)=DIAGIN*(XP(I)-SPDIAG*XP(I-1))
      YP(I)=DIAGIN*(YP(I)-SPDIAG*YP(I-1))
      SPDIAG=SINHIN*(SINHS-DELS)
      TEMP(I)=DIAGIN*SPDIAG
      DIAG1=DIAG2
   30 CONTINUE
   35 DIAGIN=1./(DIAG1-SPDIAG*TEMP(NM1))
      XP(N)=DIAGIN*(XP(N)-SPDIAG*XP(NM1))
      YP(N)=DIAGIN*(YP(N)-SPDIAG*YP(NM1))
C
C     *** PERFORM BACK SUBSTITUTION
      DO 40 I=2,N
      IBAK=NP1-I
      XP(IBAK)=XP(IBAK)-TEMP(IBAK)*XP(IBAK+1)
      YP(IBAK)=YP(IBAK)-TEMP(IBAK)*XP(IBAK+1)
   40 CONTINUE
      RETURN
   45 IF (N.EQ.2) GO TO 50
```

```
C
C     *** IF NO SLOPES ARE GIVEN, USE SECOND ORDER INTERPOLATION ON
C         INPUT DATA FOR SLOPES AT ENDPOINTS
      DELS2=SQRT((X(3)-X(2))**2+(Y(3)-Y(2))**2)
      DELS12=DELS1+DELS2
      C1=-(DELS12+DELS1)/DELS12/DELS1
      C2=DELS12/DELS1/DELS2
      C3=-DELS1/DELS12/DELS2
      SX=C1*X(1)+C2*X(2)+C3*X(3)
      SY=C1*Y(1)+C2*Y(2)+C3*Y(3)
      SLPP1=ATAN2(SY,SX)
      DELNM1=SQRT((X(N-2)-X(NM1))**2+(Y(N-2)-Y(NM1))**2)
      DELN=SQRT((X(NM1)-X(N))**2+(Y(NM1)-Y(N))**2)
      DELNN=DELNM1+DELN
      C1=(DELNN+DELN)/DELNN/DELN
      C2=-DELNN/DELN/DELNM1
      C3=DELN/DELNN/DELNM1
      SX=C3*X(N-2)+C2*X(NM1)+C1*X(N)
      SY=C3*Y(N-2)+C2*Y(NM1)+C1*Y(N)
      SLPPN=ATAN2(SY,SX)
      GO TO 10
C
C     *** IF ONLY TWO POINTS AND NO SLOPES ARE GIVEN, USE STRAIGHT
C         LINE SEGMENT FOR CURVE
   50 XP(1)=0.
      XP(2)=0.
      YP(1)=0.
      YP(2)=0.
      RETURN
C
C     *** CLOSED LOOP -- PERIODIC SPLINE -- CALCULATE SLOPES
C         FOR JOIN
   55 DELN=SQRT((X(NM1)-X(N))**2+(Y(NM1)-Y(N))**2)
      DELNN=DELS1+DELN
      C1=-DELS1/DELN/DELNN
      C2=(DELS1-DELN)/DELS1/DELN
      C3=DELN/DELNN/DELS1
      SX=C1*X(NM1)+C2*X(1)+C3*X(2)
      SY=C1*Y(NM1)+C2*Y(1)+C3*Y(2)
      IF (SX.EQ.0..AND.SY.EQ.0.) SX=1
      SLPP1=ATAN2(SY,SX)
      SLPPN=SLPP1
      GO TO 10
      END
```

SUBROUTINE KURV2

```
      SUBROUTINE KURV2 (T,XS,YS,N,X,Y,XP,YP,S,SIGMA)
C
C     THIS SUBROUTINE PERFORMS THE MAPPING OF POINTS IN THE
C     INTERVAL (0.,1.) ONTO A CURVE IN THE PLANE.  THE SUBROUTINE
C     KURV1 SHOULD BE CALLED EARLIER TO DETERMINE CERTAIN
C     NECESSARY PARAMETERS.  THE RESULTING CURVE HAS A PARAMETRIC
C     REPRESENTATION BOTH OF WHOSE COMPONENTS ARE SPLINES UNDER
C     TENSION AND FUNCTIONS OF THE POLYGONAL ARCLENGTH PARAMETER.
C
C     ON INPUT--
C     T = A REAL VALUE OF ABSOLUTE VALUE LESS THAN OR
C         EQUAL TO 1.  TO BE MAPPED TO A POINT ON THE CURVE.  THE
C         SIGN OF T IS IGNORED AND THE INTERVAL (0.,1.) IS MAPPED
C         ONTO THE ENTIRE CURVE.  IF T IS NEGATIVE THIS INDICATES
C         THAT THE SUBROUTINE HAS BEEN CALLED PREVIOUSLY (WITH ALL
C         OTHER INPUT VARIABLES UNALTERED) AND THAT THIS VALUE OF
C         T EXCEEDS THE PREVIOUS VALUE IN ABSOLUTE VALUE.  WITH
C         SUCH INFORMATION THE SUBROUTINE IS ABLE TO MAP THE POINT
C         MUCH MORE RAPIDLY.  THUS IF THE USER SEEKS TO MAP A
C         SEQUENCE OF POINTS ONTO THE SAME CURVE, EFFICIENCY IS
C         GAINED BY ORDERING THE VALUES INCREASING IN MAGNITUDE
C         AND SETTING THE SIGNS OF ALL BUT THE FIRST, NEGATIVE,
C     N = THE NUMBER OF POINTS WHICH WERE INTERPOLATED
C         TO DETERMINE THE CURVE,
C     X,Y = ARRAYS CONTAINING THE X- AND Y-COORDINATES
C         OF THE INTERPOLATED POINTS,
C     XP,YP = THE ARRAYS OUTPUT FROM KURV2 CONTAINING
C         CURVATURE INFORMATION,
C     S = THE POLYGONAL ARCLENGTH OF THE CURVE,
C     SIGMA = THE TENSION FACTOR (ITS SIGN IS IGNORED).
C
C     THE PARAMETERS N,X,Y,XP,UP,S, AND SIGMA SHOULD BE INPUT
C     UNALTERED FROM THE OUTPUT OF KURV1.
C
C     ON  OUTPUT--
C     XS,YS = THE X- AND Y-COORDINATES OF THE IMAGE
C         POINT ON THE CURVE.
C     T,N,X,Y,XP,YP,S, AND SIGMA ARE UNALTERED.
C
      DIMENSION X(N), Y(N), XP(N), YP(N)
C
C     *** DENORMALIZE SIGMA
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S
C
C     *** STRETCH UNIT INTERVAL INTO ARCLENGTH DISTANCE
      TN=ABS(T*S)
C
C     *** FOR NEGATIVE T START SEARCH WHERE PREVIOUSLY TERMINATED.
C         OTHERWISE START FROM BEGINNING
      IF (T.LT.0.) GO TO 5
      I1=2
      XS=X(1)
      YS=Y(1)
      SUM=0.
      IF (T.LE.0.) RETURN
    5 CONTINUE
C
C     *** DETERMINE INTO WHICH SEGMENT TN IS MAPPED
      DO 15 I=I1,N
      DELX=X(I)-X(I-1)
      DELY=Y(I)-Y(I-1)
      DELS=SQRT(DELX*DELX+DELY*DELY)
      IF (SUM+DELS-TN) 10,20,20
   10 SUM=SUM+DELS
   15 CONTINUE
C
C     *** IF ABS(T) IS GREATER THAN 1., RETURN TERMINAL POINT ON
C         CURVE
C
      XS=X(N)
      YS=Y(N)
      RETURN
C
C     *** SET UP AND PERFORM INTERPOLATION
   20 DEL1=TN-SUM
      DEL2=DELS-DEL1
      EXPS1=EXP(SIGMAP*DEL1)
      SINHD1=.5*(EXPS1-1./EXPS1)
      EXPS=EXP(SIGMAP*DEL2)
      SINHD2=.5*(EXPS-1./EXPS)
      EXPS=EXPS1*EXPS
      SINHS=.5*(EXPS-1./EXPS)
      XS=(XP(I)*SINHD1+XP(I-1)*SINHD2)/SINHS+((X(I)-XP(I))*DEL1+(X(I-1)-
     1XP(I-1))*DEL2)/DELS
      YS=(YP(I)*SINHD1+YP(I-1)*SINHD2)/SINHS+((Y(I)-YP(I))*DEL1+(Y(I-1)-
     1YP(I-1))*DEL2)/DELS
      I1=I
      RETURN
      END
```

SUBROUTINE FRAME

```
      SUBROUTINE FRAME (X,Y,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,FRSTY,FINY,
     1SIZY,TICY,STEPY,NDECY,LBLBOT,NB,LBLLFT,NL,LBLTOP,NT,LBLRGT,NR)
C
C     *** PURPOSE -- PREPARES AN ANNOTATED FOUR SIDED FRAME
C         WITH LOWER LEFT CORNER AT (X,Y)
C             GWL/SAI  MARCH  77
C
C         SEE SUBROUTINE AXES FOR DESCRIPTION OF ARGUMENTS
C
      COMMON /PLTVEC/ HCT(20),OT(20),NH,OHC,HCG,PLTGRD,OXN,XNG,HCC,XNC,T
     1ICZ,DIGZ,CHRZ
C
C     *** CALCULATE THE AXES LENGTHS
      XLEN=(FINX-FRSTX)*SIZX
      YLEN=(FINY-FRSTY)*SIZY
C
C     *** PLACE GRIDDED LINES ON PLOT
C
      IF (ABS(PLTGRD).EQ.0.) GO TO 40
      IF (PLTGRD.LT.0.) GO TO 25
      CALL NEWPEN (2)
      STINC=(STEPY/10.)*SIZY
      ILP=FINY/STEPY+.005
      ILP=ILP*10-1
      STVAL=STINC
      J=1
      DO 10 I=1,ILP
      IF (J.EQ.2) GO TO 5
      CALL PLOT (X,STVAL,3)
      CALL PLOT (XLEN,STVAL,2)
      STVAL=STVAL+STINC
      J=2
      GO TO 10
    5 CALL PLOT (XLEN,STVAL,3)
      CALL PLOT (X,STVAL,2)
      STVAL=STVAL+STINC
      J=1
   10 CONTINUE
      STINC=(STEPX/10.)*SIZX
      ILP=FINX/STEPX+.005
      ILP=ILP*10-1
      STVAL=STINC
      J=1
      DO 20 I=1,ILP
      IF (J.EQ.2) GO TO 15
      CALL PLOT (STVAL,Y,3)
      CALL PLOT (STVAL,YLEN,2)
      STVAL=STVAL+STINC
      J=2
      GO TO 20
   15 CALL PLOT (STVAL,YLEN,3)
      CALL PLOT (STVAL,Y,2)
      STVAL=STVAL+STINC
      J=1
   20 CONTINUE
      CALL NEWPEN (1)
      GO TO 40
C
C  PLOT GRIDDED LINES WITH MATRIX PLOTTER
C
   25 IPLT=IFIX(PLTGRD)
      CALL NEWPEN (IPLT)
      STINC=(STEPY/10.)*SIZY
      ILP=IFIX(FINY/STEPY+0.005)*10-1
      STVAL=STINC
      DO 30 I=1,ILP
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT+1)
      CALL PLOT (X+0.01,STVAL,3)
      CALL PLOT (XLEN,STVAL,2)
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT)
      STVAL=STVAL+STINC
   30 CONTINUE
      STINC=(STEPX/10.)*SIZX
      ILP=IFIX(FINX/STEPX+0.005)*10-1
      STVAL=STINC
      DO 35 I=1,ILP
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT+1)
      CALL PLOT (STVAL,Y-0.02,3)
      CALL PLOT (STVAL,Y,3)
      CALL PLOT (STVAL,YLEN,2)
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT)
      STVAL=STVAL+STINC
   35 CONTINUE
      CALL NEWPEN (0)
   40 CONTINUE
C
C     *** PLOT THE FOUR SIDES WITH ANNOTATIONS
      CALL AXES (X,Y,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,0.,LBLBOT,-NB,1)
      CALL AXES (X,Y,FRSTY,FINY,SIZY,TICY,STEPY,NDECY,90.,LBLLFT,NL,1)
      CALL AXES (X,Y+YLEN,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,0.,LBLTOP,NT,
     1-1)
      CALL AXES (X+XLEN,Y,FRSTY,FINY,SIZY,TICY,STEPY,NDECY,90.,LBLRGT,-N
     1R,-1)
C
      RETURN
      END
```

SUBROUTINE AXES

```
      SUBROUTINE AXES (X,Y,FIRSTV,FINALV,SCALE,TSTEP,ASTEP,NDEC,ANGLE,IB
     1CD,NCHAR,LABEL)
C
C     *** SAI SUBROUTINE AXES
C         GW LUNDBERG/SAI  DEC 76
C
C         X,Y = COORDINATES IN INCHES OF AXIS LINE STARTING
C               POINT
C         FIRSTV = STARTING VALUE FOR THE AXIS
C         FINALV = ENDING VALUE FOR THE AXIS
C         SCALE = INCHES/UNIT FOR FIRSTV,FINALV,TSTEP,ASTEP
C         TSTEP = STEP SIZE FOR TICS
C         ASTEP = STEP SIZE FOR LABELED TICS
C         NDEC = FORMAT FOR LABELS -- SEE SUBROUTINE NUMBER
C         ANGLE = ANGLE OF AXIS IN DEGREES FROM HORIZONTAL
C         IBCD = THE AXIS TITLE AS ARRAY OR HOLLERITH STRING
C         NCHAR = NUMBER OF CHARACTERS IN TITLE
C               ) 0, TIC MARKS, ANNOTATION AND TITLE PLOTTED ON
C                   CLOCKWISE SIDE OF AXIS LINE
C               ( 0, ON COUNTER CLOCKWISE SIDE
C
C         THIS ROUTINE WAS WRITTEN FOR A MATRIX PLOTTER -- IT DOES
C         NOT OPTIMIZE PEN MOVEMENTS.  THE ROUTINE SHOULD BE MACHINE
C         INDEPENDENT
C
C
C     *** FOLLOWING ARE ADJUSTABLE -- IF LABEL ) 0, ALL TICS ARE
C         LABELED, IF LABEL = 0, THE LAST TIC IS NOT LABELED,
C         IF LABEL ( 0, THE FIRST AND LAST ARE NOT LABELED
C
C     *** DEFINE VARIOUS CHARACTER SIZES
      COMMON /PLTVEC/ HCT(20),OT(20),NH,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICSIZ,DIGSIZ,CHRSIZ
C
C     *** STEP 1 -- DRAW AXIS AND TIC MARKS
C         ---- -    ---- ---- --- --- -----
C
C     *** MOVE PEN TO START OF AXIS
      X0=X
      Y0=Y
      CALL PLOT (X0,Y0,3)
C
C     *** LOCATE THE OTHER END AND DRAW AXIS
      COSA=COS(ANGLE*0.017453294)
      SINA=SIN(ANGLE*0.017453294)
      AXLEN=(FINALV-FIRSTV)*SCALE
      X1=X0+AXLEN*COSA
      Y1=Y0+AXLEN*SINA
      CALL PLOT (X1,Y1,2)
C
C     *** ADD THE TIC MARKS ON WRONG SIDE OF AXIS
      POS=FLOAT(ISIGN(1,NCHAR))
      IF (TSTEP.EQ.0.) GO TO 10
      NTIC=(FINALV-FIRSTV)/TSTEP+1.5
      DO 5 J=1,NTIC
C
C         *** MOVE PEN TO START OF TIC
      X1=X0+FLOAT(J-1)*TSTEP*SCALE*COSA
      Y1=Y0+FLOAT(J-1)*TSTEP*SCALE*SINA
      CALL PLOT (X1,Y1,3)
C
C         *** DRAW A TIC NORMAL TO AXIS
      X1=X1+TICSIZ*POS*SINA
      Y1=Y1-TICSIZ*POS*COSA
      CALL PLOT (X1,Y1,2)
    5 CONTINUE
C
C     *** STEP 2 -- SET IN LABELED TICS ON CORRECT SIDE OF AXIS
C         ---- -    --- -- ------- ---- -- ------- ---- -- ----
C
```

```
   10 IF (ASTEP.EQ.0.) GO TO 25
      NTIC=(FINALV-FIRSTV)/ASTEP+1.5
      NFRST=1
      NLST=NTIC
      IF (LABEL.LE.0) NLST=NLST-1
      IF (LABEL.LT.0) NFRST=NFRST+1
      DO 15 J=NFRST,NLST
      X1=X0+FLOAT(J-1)*ASTEP*SCALE*COSA
      Y1=Y0+FLOAT(J-1)*ASTEP*SCALE*SINA
      CALL PLOT (X1,Y1,3)
C
      X1=X1-TICSIZ*POS*SINA
      Y1=Y1+TICSIZ*POS*COSA
      CALL PLOT (X1,Y1,2)
   15 CONTINUE
C
C     *** STEP 3 -- ANNOTATE THE TIC MARKS
C         ---- -    -------- --- --- -----
C
C     *** DETERMINE PERPENDICULAR OFFSET TO BOTTOM OF CHARACTER
      OFFSET=TICSIZ+0.03
      IF (POS.NE.1) OFFSET=OFFSET+DIGSIZ
C
C     *** CALCULATE LOCATION OF FIRST CHARACTER
      X0=X0-DIGSIZ*COSA
      Y0=Y0-DIGSIZ*SINA
      X0=X0-OFFSET*POS*SINA
      Y0=Y0+OFFSET*POS*COSA
C
C     *** ANNOTATE THE TIC MARKS
      NFRST=1
      NLAST=NTIC
      IF (LABEL.LE.0) NLAST=NLAST-1
      IF (LABEL.LT.0) NFRST=NFRST+1
      DO 20 J=NFRST,NLAST
C
C         *** GET FLOATING POINT VALUE OF ANNOTATION
      FPN=FIRSTV+FLOAT(J-1)*ASTEP
C
C         *** GET LOCATION AND PLOT FPN
      X1=X0+FLOAT(J-1)*ASTEP*SCALE*COSA
      Y1=Y0+FLOAT(J-1)*ASTEP*SCALE*SINA
      CALL NUMBER (X1,Y1,DIGSIZ,FPN,ANGLE,NDEC)
   20 CONTINUE
C
C     *** STEP 4 -- ADD AXIS TITLE
C         ---- -    --- ---- -----
C
   25 IF (NCHAR.EQ.0) GO TO 30
C     *** SET TITLE OFFSET -- DISTANCE FROM AXIS TO CHARACTERS
      OFFSET=TICSIZ+DIGSIZ+0.10
      IF (NCHAR.LT.0) OFFSET=OFFSET+CHRSIZ
C
C     *** CALCULATE TITLE SIZE
      TSIZ=CHRSIZ*IABS(NCHAR)
C
C     *** CALCULATE OFFSET FROM BEGINNING OF AXIS TO FIRST CHARACTER
      OFF=0.5*(AXLEN-TSIZ)
C
C     *** CALCULATE LOCATION OF FIRST CHARACTER AND PLOT TITLE
      X0=X+OFF*COSA
      Y0=Y+OFF*SINA
      X0=X0-OFFSET*POS*SINA
      Y0=Y0+OFFSET*POS*COSA
      CALL SYMBOL (X0,Y0,CHRSIZ,IBCD,ANGLE,IABS(NCHAR))
C
C         FINISHED
   30 RETURN
      END
```

SUBROUTINE CCMIX

```
      SUBROUTINE CCMIX
      COMMON /SUNLIT/ XJ(47,10),SIGMO(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(16),XZ(16),K(16),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL,MA
     3XJ
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /MIXING/ DSTRT,DEND,A(5),B(5),C(5),FD(6),
     1Y(6),AMIX(16),DL,TTMAX,SRISE,HMIN,DELH,TDIL,NMIX
C
C --- DETERMINE TIME OF SUNRISE (STANDARD TIME)
C
      T=400.
   10 CALL SOLAR(SLA,SLO,TZ,IY,IM,ID,T,D,5)
      IF(D.GE.1.) GO TO 15
      T=CLOCK(T,5)
      GO TO 10
C
C --- CONVERT SUNRISE TO LOACL DAYLIGHT TIME
C
   15 TSR=CLOCK(T,60)
      IF(TSR.LT.0600.) TSR=0600.
C
C --- DETERMINE SOLAR DECLINATION AND DAY LENGTH
C
      CALL SOLAR(SLA,SLO,TZ,IY,IM,ID,1200.,D,1)
      D=D*3.14159/180.
      ARG1=-TAN(0.67399)*TAN(D)
      DL=ACOS(ARG1)/3.14159*1440.
      IDL=DL
      TSS=CLOCK(TSR,IDL)
C
C --- COMPUTE TIME MAXIMUM HEIGHT IS REACHED
C
      TMAX=.70*DL
      ITMAX=TMAX
      TTMAX=CLOCK(TSR,ITMAX)
C
C --- CONVERT ALL 2400 HOUR TIMES TO MINUTES AFTER SUNRISE
C
      SRISE=(IFIX(TSR/100.)*60.)+(TSR-(IFIX(TSR/100.)*100.))
      DDSTRT=(IFIX(DSTRT/100.)*60.)+(DSTRT-(IFIX(DSTRT/100.)*100.))
      DDEND=(IFIX(DEND/100.)*60.)+(DEND-(IFIX(DEND/100.)*100.))
      DDSTRT=DDSTRT-SRISE
      DDEND=DDEND-SRISE
C
C --- COMPUTE HMIN AND DELTA HEIGHT
C
      FD1=DDSTRT/DL
      FD2=DDEND/DL
      DO 40 J=1,5
      IF(FD1.GE.FD(J).AND.FD1.LT.FD(J+1)) II=J
      IF(FD2.GE.FD(J).AND.FD2.LT.FD(J+1)) JJ=J
   40 CONTINUE
      IF(FD1.GE.0.0) GO TO 25
      FD1=0.0
      II=1
   25 IF(FD2.LT.0.70) GO TO 20
      FD2=.7
      JJ=6
   20 CONTINUE
      X=FD1-FD(II)
      XX=FD2-FD(JJ)
      FG1=((A(II)*X+B(II))*X+C(II))*X+Y(II)
      FG2=((A(JJ)*XX+B(JJ))*XX+C(JJ))*XX+Y(JJ)
      DELH=(Z2-Z1)/(FG2-FG1)
      HMIN=Z1-FG1*DELH
      HMAX=HMIN+DELH
C
C --- COMPUTE MIXING HEIGHTS AT HOURLY INTERVALS
```

```
C
      NMIX=0
      JJSTP=JSTOP-100
      IT=JSTRT/100
      T=IT*100
      IF(DEND.GT.TTMAX) DEND=TTMAX
      DO 70 J=1,16
      IF(T.LT.DSTRT) GO TO 55
      IF(T.GE.DEND) GO TO 60
      TT=(IFIX(T/100.)*60.)+(T-(IFIX(T)/100.)*100.)
      TT=TT-SRISE
      FDT=TT/DL
      IF(FDT.LT.0.0) FDT=0.0
      KK=0
   45 KK=KK+1
      IF(FDT.GE.FD(KK).AND.FDT.LT.FD(KK+1)) GO TO 50
      IF(KK.LT.5) GO TO 45
      IF(FDT.GE.FD(6)) GO TO 60
   50 CONTINUE
      X=FDT-FD(KK)
      FG=((A(KK)*X+B(KK))*X +C(KK))*X+Y(KK)
      AMIX(J)=HMIN+FG*DELH
      NMIX=NMIX+1
      IF(T.GE.JJSTP) GO TO 80
      GO TO 65
   55 AMIX(J)=Z1
      NMIX=NMIX+1
      GO TO 65
   60 AMIX(J)=Z2
      NMIX=NMIX+1
      GO TO 80
   65 CONTINUE
      T=T+100.
   70 CONTINUE
   80 CONTINUE
C
C --- SETUP DILUTION TIMES FOR SIMULATION CONTROL
C
      JMIN=IFIX(DSTRT)-((IFIX(DSTRT)/100)*100)
      TMIN1=FLOAT((IFIX(DSTRT)/100)*60+JMIN)
      JMIN=IFIX(DEND)-((IFIX(DEND)/100)*100)
      TMIN2=FLOAT((IFIX(DEND)/100)*60+JMIN)
      JMIN=JSTRT-((JSTRT/100)*100)
      TMIN3=FLOAT((JSTRT/100)*60+JMIN)
      TMIN4=AMAX1(TMIN1,TMIN3,SRISE)
      TSRT=TMIN4-TMIN3
      IF (TSRT.GT.0.) DTIM=TMIN2-TMIN4
      IF (TSRT.LE.0.) DTIM=TMIN2-TMIN3
      IF (DTIM.LT.0.) DTIM=0.
      RETURN
      END
```

SUBROUTINE EKMA

```
      SUBROUTINE EKMA
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /SUPPR/NOPR
      COMMON/EKMART/BCO3,BCRAT,DELNOX,ICHTRN,IRANGE,FOZIN,FOZAL,FHCIN,
     1FHCAL,FXNIN,FXNAL
      NOPR=1
      ERRTOL=.0005
      WRITE(IOUT,200)
      WRITE(IOUT,210) OZIN,OZAL,HCIN,HCAL,XNIN,XNAL
      WRITE(IOUT,220) FOZIN,FOZAL,FHCIN,FHCAL,FXNIN,FXNAL
      WRITE(IOUT,230) DELNOX
      WRITE(IOUT,240)
      XHC=1.0
      XNOX=1.0/BCRAT
      CALL SIM(XHC,XNOX,PREDO3,1)
      INUM=1
      WRITE(IOUT,250) INUM,XHC,XNOX,BCRAT,PREDO3,BCO3
      POINT2=XHC
      SIMNOX=XNOX
      ZN2=PREDO3
      IF(ABS(BCO3-PREDO3).LT.ERRTOL) GO TO 30
C
C***  CALCULATE SECOND GUESS FOR MAX OZONE
C
      A=(PREDO3-BCO3)/BCO3+1
      POINT2=XHC/A
      POINT1=XHC
      ZN1=PREDO3
C
C***  SUCCESSIVE APPROXIMATION OF MAX OZONE ON XHC/XNOX LINE
C
    5 DO 20 I=1,9
      SIMNOX=POINT2/BCRAT
      INUM=INUM+1
      CALL SIM (POINT2,SIMNOX,ZN2,1)
      WRITE(IOUT,250) INUM,POINT2,SIMNOX,BCRAT,ZN2,BCO3
      IF (ABS(BCO3-ZN2).LT.ERRTOL) GO TO 30
      PNTNEW=POINT1+(BCO3-ZN1)*(POINT2-POINT1)/(ZN2-ZN1)
      IF(PNTNEW.LT.0.0) PNTNEW=0.10
      POINT1=POINT2
      ZN1=ZN2
      POINT2=PNTNEW
   20 CONTINUE
C
C***  UNSUCCESSFUL APPROXIMATION OF MAX OZONE, PRINT MSG, EXIT
C
      WRITE (IOUT,11)
      RETURN
   30 CONTINUE
      HC1=POINT2
      WRITE(IOUT,260) HC1
C
C***  PRIOR TO CALCULATING HC & NOX FOR .12 OZONE,
C***  CALCULATE REVISED TRANSPORT CONCENTRATIONS
C
      IF(ICHTRN.EQ.0) GO TO 35
      OZSFC=OZIN
      OZUPP=OZAL
      HCSFC=HCIN
      HCUPP=HCAL
      XNSFC=XNIN
      XNUPP=XNAL
      OZIN=FOZIN
      OZAL=FOZAL
      HCIN=FHCIN
      HCAL=FHCAL
      XNIN=FXNIN
      XNAL=FXNAL
   35 CONTINUE
C
C***  CALCULATE FIRST GUESS FOR .12 OZONE
C
      GOAL=0.12
      POINT1=POINT2
      ZN1=ZN2
      CTLNOX=SIMNOX*(1.+DELNOX/100.)
      POINT2=GOAL*HC1/ZN1
      WRITE(IOUT,270)
C
C***  SUCCESSIVE APPROXIMATION OF .12 OZONE FOR CONSTANT NOX
C
      INUM=0
      DO 40 I=1,10
      INUM=INUM+1
      CALL SIM (POINT2,CTLNOX,ZN2,1)
      WRITE(IOUT,280) INUM,POINT2,CTLNOX,ZN2,GOAL
      IF (ABS(GOAL-ZN2).LT.ERRTOL) GO TO 50
      PNTNEW=POINT1+(GOAL-ZN1)*(POINT2-POINT1)/(ZN2-ZN1)
      IF(PNTNEW.LT.0.0) PNTNEW=0.10
      POINT1=POINT[illegible]
      ZN1=ZN2
      POINT2=PNTNEW
   40 CONTINUE
C
C***  UNSUCCESSFUL APPROXIMATION OF .12 OZONE, EXIT
C
      WRITE (IOUT,13)
      RETURN
   50 CONTINUE
      WRITE(IOUT,290) POINT2
C
C***  CALCULATE, PRINT % REDUCTION
C
      IBASE=IFIX((HC1*100.)+0.5)
      HC1=FLOAT(IBASE)/100.
      IBASE=IFIX((POINT2*100.)+0.5)
      POINT2=FLOAT(IBASE)/100.
      REDUC=(1.-POINT2/HC1)*100.
      IRED=IFIX(REDUC+0.5)
      WRITE (IOUT,300) IRED
      IF(IRANGE.GT.0.) CALL RANGE(HC1,CTLNOX,DELNOX,BCO3,IRANGE)
C
C***  RETURN TRANSPORTED OZONE CONCENTECRATNS TO ORIGINAL VALUES
C
      IF(ICHTRN.EQ.0) GO TO 60
      OZIN=OZSFC
      OZAL=OZUPP
      HCIN=HCSFC
      HCAL=HCUPP
      XNIN=XNSFC
      XNAL=XNUPP
   60 CONTINUE
      NOPR=0
      RETURN
C
C***  FORMATS
C
   11 FORMAT (1X,'UNABLE TO FIND MAX OZONE IN 10 TRIES, EXITING.')
   13 FORMAT (1X,'UNABLE TO FIND OZONE GOAL IN 10 TRIES, EXITING.')
  200 FORMAT(1H1,'EKMA HC REDUCTION CALCULATION'///)
  210 FORMAT(1X,'TRANSPORTED CONCENTRATIONS'//,
     11X,24X,3('SURFACE',2X,'ALOFT',3X)/
     21X,25X,'OZONE',3X,'OZONE',6X,'HC',6X,'HC',6X,'NOX',5X,'NOX'//
     36X,'PRE-CONTROL',9X,F5.3,3X,F5.3,4X,F5.3,3X,F5.3,4X,F5.3,3X,F5.3/)
  220 FORMAT(6X,'POST-CONTROL',8X,F5.3,3X,F5.3,4X,F5.3,3X,F5.3,4X,F5.3,
     13X,F5.3)
  230 FORMAT(//1X,'PERCENT NOX CHANGE BETWEEN PRE- AND POST-'
    1,'CONTROL:',F5.1)
240 FORMAT(//1X,'ITERATIONS FOR PRE-CONTROL POINT:'//
    18X,'INITIAL',2X,'INITIAL',2X,'HC/NOX',2X,'PREDICTED',2X
    2,'PRE-CONTROL'/,2X,'NUM',5X,'HC',7X,'NOX',5X,'RATIO',4X
    3,'OZONE',7X,'OZONE'/)
250 FORMAT(2X,I2,4X,F5.2,4X,F5.3,4X,F5.1,4X,F6.4,6X,F6.4)
260 FORMAT(/6X,'***PRE-CONTROL HC =',1X,F5.2)
270 FORMAT(//1X,'ITERATIONS FOR POST-CONTROL POINT:'//
    18X,'INITIAL',2X,'INITIAL',3X,'PREDICTED',3X,'POST-CONTROL'/
    22X,'NUM',5X,'HC',7X,'NOX',7X,'OZONE',8X,'OZONE'/)
280 FORMAT(2X,I2,4X,F5.2,4X,F5.3,6X,F6.4,7X,F6.4)
290 FORMAT(/6X,'***POST-CONTROL HC =',1X,F5.2)
300 FORMAT(///10X,'EKMA HC REDUCTION =',1X,I4,'%')
    END
```

SUBROUTINE RANGE

```
      SUBROUTINE RANGE(HC1,CTLNOX,DELNOX,OZ1,IRANGE)
      COMMON /INOUT/ IN,IOUT,ITAPE
      DIMENSION OZOUT(11)
      WRITE(IOUT,5)
      WRITE(IOUT,10)
      DELHC=10.0
      DO 100 K=1,11
      DELHC=DELHC-10.
      HC2=HC1*(1.0+DELHC/100.)
      CALL SIM(HC2,CTLNOX,ZN,1)
      DELO3=((ZN-OZ1)/OZ1)*100.
      WRITE(IOUT,20) HC2,CTLNOX,ZN,DELHC,DELNOX,DELO3
      OZOUT(K)=ZN
  100 CONTINUE
      IF (IRANGE.EQ.2) WRITE(11,30) OZOUT
      RETURN
    5 FORMAT(1H1,'EKMA PREDICTED CHANGES IN OZONE')
   10 FORMAT(///12X,'HC',6X,'NOX',6X,'O3',4X,'%-CHG HC',3X,
     *'%-CHG NOX',3X,'%-CHG O3'/)
   20 FORMAT(10X,F6.3,3X,F5.3,3X,F5.4,4X,F6.1,5X,F6.1,
     *6X,F6.1)
   30 FORMAT(11F5.3)
      END
```

FUNCTION CIRC

```
      FUNCTION CIRC (TI,XI,YI)
      DIMENSION XI(3), YI(3)
      DX=XI(3)-XI(1)
      DY=YI(3)-YI(1)
      X=(XI(2)-XI(1))/DX
      Y=(YI(2)-YI(1))/DY
      T=(TI-XI(1))/DX
      IF (X.EQ.Y) GO TO 10
      B=((X*X+Y*Y)*0.5-X)/(Y-X)
      TT=SQRT(B*B+2.*T*(1.-B)-T*T)
      CX=B+TT
      IF (X.GT.Y) CX=B-TT
      IF (CX.LT.0..OR.CX.GT.1.) GO TO 10
    5 CIRC=CX*DY+YI(1)
      RETURN
   10 CX=T*Y/X
      IF (T.GT.X) CX=(T-X)*(1.-Y)/(1.-X)+Y
      GO TO 5
      END
```

SUBROUTINE EMISS

```
      SUBROUTINE EMISS (N,H,COEFF)
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C TO HANDLE MORE THAN 16 HISTOGRAM INTERVALS (ASSUMING N IS #INTERVALS)
C THE DIMENSIONED VARIABLES BELOW MUST HAVE THE FOLLOWING DIMENSIONS
C H = N; Y,DYDX = N+1; CF,COEFF = 5*N
C SEE ALSO DIMENSION STATEMENT IN STAIR
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
        DIMENSION H(16), CF(80), Y(17), DYDX(17), COEFF(80)
        REAL*8 CF, Y, DYDX, HRATIO, EXPONE, FORRAT, FORCDY, RATLIM
        REAL*8 SIGNDY, SMALLV
        REAL DELX, H, COEFF
        INTEGER STARTY, STOPY, INDEX, N, MODE, MODE1I
        INTEGER NPLUS1, FIVEN, J, K
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C   N IS THE NUMBER OF HISTOGRAM INTERVALS
C   N + 1  IS THE NUMBER OF EDGES IN THE HISTOGRAM PLOT
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
        RATLIM= 5.001
        MODE=1
        DELX=1.0
        FORRAT= 2.5
        FORCDY = 5.25
        NPLUS1 = N + 1
        FIVEN = 5 * N
        IF ( FIVEN .LE. 1) GO TO 45
        DO 40 J = 1 , FIVEN
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C   SET ALL COEFFICIENTS TO ZERO IN THE CF ARRAY.
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
          CF(J) = 0.0
   40   CONTINUE
   45   CONTINUE
        IF ( NPLUS1 .LE. 1) GO TO 55
        DO 50 J = 1 , NPLUS1
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  ZERO OUT ALL THE Y'S AND DYDX'S,  IN THE PROCESS
C    FORCING THE EDGE OF THE LAST DELX INTERVAL TO ZERO
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
          Y(J) = 0.0
          DYDX(J) = 0.0
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  LOOK FOR THE FIRST NON-ZERO H
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
   50   CONTINUE
   55   CONTINUE
        INDEX = 1
C       WHILE ((H(INDEX) .LE. 0.0) .AND. (INDEX .LT. N))
   60   IF ((H(INDEX) .GT. 0.0) .OR. (INDEX .GE. N)) GO TO 65
          INDEX = INDEX + 1
        GO TO 60
   65   CONTINUE
        STARTY = INDEX
        INDEX = INDEX + 1
        MODE1I = 1
C       IF (MODE .NE. 0)
        IF (MODE .EQ. 0) GO TO 70
C        THEN
          MODE1I = STARTY
          Y(STARTY) = H(STARTY)
          DYDX(STARTY) =  0.0
   70   CONTINUE
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  STAIR DETERMINES THE COEFFICIENTS OF THE FOURTH DEGREE
C  POLYNOMIAL F(X)= (((AX+B)X+C)X+D)X+E SUCH THAT F(X) IS
C  TWICE DIFFERENTIABLE ACROSS HISTOGRAM INTERVAL EDGES,
C  MATCHES IN VALUE AT THE INTERVAL EDGES, AND SUCH THAT
C  THE INTEGRAL OF F(X)DX = THE HISTOGRAM INTERVAL HEIGHT
C  TIMES THE INTERVAL WIDTH (DELX). THE CROSSOVER POINTS
C  (THE VALUES OF F(X) AT THE EDGES BETWEEN TWO HISTOGRAM
C  INTERVALS) ARE THE KNOWNS. STAIR SOLVES FOR THE VALUES
C  OF F'(X) AT THE EDGES GIVEN THE BOUNDARY CONDITIONS OF
C  F'(X) AT THE TWO ENDS OF EACH STAIR EVALUATION. HISFIT
C  STEPS THROUGH THE HISTOGRAM IN ONE PASS, BREAKING THE
C  HISTOGRAM INTO STAIR EVALUATIONS OF 1 OR MORE INTERVALS.
C  NOTE THAT THE CURVE DEFINED BY THE COEFFICIENTS IS ONLY
C  ONCE DIFFERENTIABLE AT EDGES BETWEEN STAIR EVALUATIONS.
C  STAIR EVALUATIONS MAY NOT CROSS POINTS WHERE F'(X) IS
C  KNOWN OR FIXED E.G. ZERO POINTS (DY/DX = 0), OR FORCE
C  FITS (WHERE UNRESTRAINED STAIR FITS RESULT IN FUNCTIONS
C  WITH NEGATIVE VALUES WHICH CORRESPONDS TO NO PHYSICAL
C  REALITY). AT THESE EDGES, THE CURRENT STAIR EVALUATION
C  IS TERMINATED AND A NEW STAIR EVALUATION STARTED. IF
C  THE RATIO OF ADJACENT HISTOGRAM VALUES IS LESS THAN 5/1
C  A CROSSOVER POINT IS PICKED ACCORDING TO THE HEURISTIC:
C         Y =  (RATIO ** 0.50)*(SMALLER VALUE)
C  WHERE 5.001 .GT. RATIO .GT. 1. FOR THE SPECIAL CASE OF A VALUE
C  WHICH HAS A ZERO VALUE TO ONE SIDE, THE OTHER EDGE
C  CROSSOVER IS: Y =  (RATIO ** 0.57)*(SMALLER VALUE)
C  WHERE 5.001 .GT. RATIO .GT. 1. IF THE RATIO OF ADJACENT
C  HISTOGRAM VALUES EXCEEDS 5 A FIT IS FORCED BY APPROX-
C  IMATING A RATIO-OF-5 FIT THROUGH THE SMALLER VALUE.
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C       WHILE (INDEX .LE. N)
   90   IF (INDEX .GT. N) GO TO 95
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  STEP THROUGH HISTOGRAM, BREAK INTO STAIR EVALUATIONS
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C         IF (H(INDEX) .LE. 0.0)
          IF (H(INDEX) .GT. 0.0) GO TO 100
C          THEN
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C CASE OF NEGATIVE OR ZERO HEIGHT
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
            STOPY = INDEX
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C FIT A SPLINE TO THIS POINT
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
            CALL STAIR(STARTY,STOPY,DELX,H,Y,DYDX,CF)
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C LOOK FOR NEXT NON ZERO H
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C           WHILE ((H(INDEX) .LE. 0.0) .AND. (INDEX .LT. N))
  120       IF ((H(INDEX) .GT. 0.0) .OR. (INDEX .GE. N))
     1         GO TO 125
              INDEX = INDEX + 1
            GO TO 120
  125       CONTINUE
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C START NEW STAIR EVALUATION
```

```
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
            STARTY = INDEX
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  GOTO BOTTOM OF LOOP
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
            GO TO 105
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  IT IS GUARANTEED THAT H(INDEX-1) AND H(INDEX) ARE .GT. 0.0
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
  100      CONTINUE
C          ELSE
            HRATIO = H(INDEX) / H(INDEX-1)
            EXPONE= 0.50
C           IF (HRATIO .GE. 1.0)
            IF (HRATIO .LT. 1.0) GO TO 140
C            THEN
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  BEGIN UP STEP
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
              SIGNDY = 1.0
              SMALLV= H(INDEX-1)
C             IF ((INDEX .EQ. (MODE1I + 1)) .AND. (MODE .EQ. 0))
              IF ((INDEX .NE. (MODE1I + 1)) .OR. (MODE .NE. 0))
     1           GO TO 160
C              THEN
                EXPONE = 0.57
                GO TO 165
  160          CONTINUE
C              ELSE
C               IF .NOT.((INDEX .EQ. 2) .AND. (MODE .NE. 0))
                IF ((INDEX .EQ. 2) .OR. (MODE .NE. 0)) GO TO 170
C                THEN
C                 IF (H(INDEX-2) .EQ. 0.0)
                  IF (H(INDEX-2) .NE. 0.0) GO TO 180
C                  THEN
                    EXPONE = 0.57
  180             CONTINUE
  170           CONTINUE
  165         CONTINUE
              GO TO 185
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  END UP STEP
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
  140        CONTINUE
C            ELSE
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  BEGIN DOWN STEP
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
              HRATIO = 1.0 / HRATIO
              SIGNDY = -1.0
              SMALLV= H(INDEX)
C             IF (INDEX .EQ. N)
              IF (INDEX .NE. N) GO TO 190
C              THEN
                EXPONE = 0.57
                GO TO 195
  190          CONTINUE
C              ELSE
C               IF (H(INDEX+1) .EQ. 0.0)
```

```
               IF (H(INDEX+1) .NE. 0.0) GO TO 200
C               THEN
                 EXPONE = 0.57
  200          CONTINUE
  195        CONTINUE
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  END DOWN STEP
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
  185       CONTINUE
C           IF (HRATIO .LT. RATLIM)
            IF (HRATIO .GE. RATLIM) GO TO 205
C            THEN
              Y(INDEX) = (HRATIO ** EXFONE) * SMALLV
              GO TO 210
C            ELSE
  205        CONTINUE
              Y(INDEX) = FORRAT * SMALLV
              DYDX(INDEX) = SIGNDY * FORCDY * (Y(INDEX) / DELX)
              STOPY = INDEX
              CALL STAIR(STARTY,STOPY,DELX,H,Y,DYDX,CF)
              STARTY = INDEX
  210      CONTINUE
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  BOTTOM OF LOOP, EXAMINE NEXT INTERVAL
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
  105     CONTINUE
          INDEX = INDEX + 1
        GO TO 90
   95   CONTINUE
C       ENDWHILE (INDEX .LE. N) LOOP
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  FOR THE FINAL SPLINE PORTION, CALL STAIR.
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C       IF (STARTY .NE. (N+1)) .AND. (H(N) .NE. 0.0)
        IF ((STARTY .EQ. (N+1)) .OR. (H(N) .EQ. 0.0))
     1     GO TO 220
C        THEN
          STOPY = N + 1
          CALL STAIR(STARTY,STOPY,DELX,H,Y,DYDX,CF)
  220   CONTINUE
        IF (1 .GT. FIVEN) GO TO 255
        DO 260 K = 1 , FIVEN
          COEFF(K) = CF(K)
  260   CONTINUE
  255   CONTINUE
      RETURN
      END
```

SUBROUTINE CONVT

```
      SUBROUTINE CONVT (NUM,L)
C
C    SUBROUTINE CONVT CONVERTS INTEGERS TO ALPHANUMERIC FOR
C  PRINTING
C
C  ASSUMES VALUE OF INTEGER IS POSITIVE
C
      DIMENSION L(3), JDIGIT(10)
C
      DATA JDIGIT/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/
      DATA JBLANK/1H /
C
      N=NUM
      DO 5 I=1,3
      L(I)=JBLANK
    5 CONTINUE
C
      DO 10 K=1,3
      I=4-K
      NEXT=N/10
      NDX=(N-NEXT*10)+1
      L(I)=JDIGIT(NDX)
      NK=K
      IF (NEXT.LE.0) GO TO 15
      N=NEXT
   10 CONTINUE
C
C
   15 RETURN
      END
```

SUBROUTINE EDGMX

```
      SUBROUTINE EDGMX (X,Y,N,XMX,YMX,L)
      DIMENSION X(N), Y(N)
      LL=N-1
      IF (N.LE.2) GO TO 10
      NGO=0
      DO 5 I=2,LL
      IF (Y(I).GT.Y(I-1)) GO TO 5
      IF (Y(I).GT.Y(I+1)) L=I+1
      IF (Y(I).GT.Y(I+1)) NGO=1
      GO TO 6
    5 CONTINUE
    6 CONTINUE
      IF (NGO.EQ.1) GO TO 15
   10 XMX=X(N)
      YMX=Y(N)
      L=N-1
      RETURN
   15 L=MAX0(L-1,3)
      X21=X(L-1)-X(L-2)
      X221=X(L-1)*X(L-1)-X(L-2)*X(L-2)
      X32=X(L)-X(L-1)
      XL2=X(L)*X(L)
      Y21=Y(L-1)-Y(L-2)
      C=(Y21/X21-(Y(L)-Y(L-1))/X32)/(X221/X21-(XL2-X(L-1)*X(L-1))/X32)
      B=(Y21-C*X221)/X21
      A=Y(L)-B*X(L)-C*XL2
      XMX=-B*0.5/C
      YMX=A+B*XMX+C*XMX*XMX
      IF (XMX.GE.0.999*X(L)) YMX=Y(L)
      IF (YMX.EQ.Y(L)) XMX=X(L)
      IF (XMX.LT.1.001*X(L-2).AND.L.GT.3) GO TO 15
      L=L-1
      IF (XMX.LE.X(L)) L=L-1
      RETURN
      END
```

SUBROUTINE STAIR

```
      SUBROUTINE STAIR(KSTRT,KSTOP,DELX,H,Y,DYDX,CF)
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C TO HANDLE MORE THAN 16 HISTOGRAM INTERVALS (ASSUMING N IS #INTERVALS)
C THE DIMENSIONED VARIABLES BELOW MUST HAVE THE FOLLOWING DIMENSIONS
C H = N; Y,DYDX,A,B,C = N+1; CF = 5*N
C SEE ALSO DIMENSION STATEMENT IN HISFIT
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
        DIMENSION A(17), B(17), C(17), CF(80), Y(17), DYDX(17), H(16)
        REAL*8 A, B, C, R, S1, S2, T1, T2, U1, U2, V1, V2, Z
        REAL*8 Y, DYDX, CF
        REAL DELX, H
        INTEGER K,KSTRT,KSTOP,KSTOP1, J1, J2
        INTEGER KSTOP2, KDOWN, KSTRT1
        KSTOP1 = KSTOP - 1
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  COMPUTE COEFFICIENTS FOR
C   FK(X)=AK(X-XK)4 + BK(X-XK)3 + CK(X-XK)2 + DK(X-XK) +EK
C
C  STORE IN ARRAY CF AS:
C    CF 5*K =A;        CF 5*K-1 =B;       CF 5*K-2 =C;
C    CF 5*K-3 =D=YKP                      CF 5*K-4 =E=YK
C    CF 5*K-3 =D=YKP                      CF 5*K-4 =E=YK
C     FOR K=KSTRT TO KSTOP  (WHERE KSTOP-KSTRT IS THE NUMBER
C                                OF INTERVALS. )
C   KSTRT  IS THE LEFT EDGE OF THE STARTING HISTOGRAM BAR
C   KSTOP  IS THE RIGHT EDGE OF THE STOPPING HISTOGRAM BAR
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
        IF (KSTRT .GT. KSTOP1) GO TO 300
        DO 295 K = KSTRT , KSTOP1
          CF(5*K-4)=Y(K)
  295   CONTINUE
  300   CONTINUE
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C SET UP AND SOLVE MATRIX
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
        B(KSTRT)=0.0
        C(KSTRT)=0.0
        IF ( KSTRT .GT. KSTOP1) GO TO 310
        DO 305 K = KSTRT , KSTOP1
          J2=K+1
          U2=1.0/(DELX)
          A(K)=U2
          V2=U2*U2
          S2=20.0*V2*H(K)
          T2=8.0*V2*(Y(K)+Y(J2))
C         IF (K.GT.KSTRT)
          IF (K.LE.KSTRT) GO TO 315
C          THEN
            Z=1.0/(3.0*(U1+U2)+U1*B(J1))
            B(K)= -U2*Z
            R=S2-S1-T2+T1+4.0*(V1-V2)*Y(K)
C           IF (K.EQ.KSTRT+1)
            IF (K.NE.KSTRT+1) GO TO 335
C            THEN
              R=R+U1*DYDX(KSTRT)
  335       CONTINUE
C           IF (K.EQ.KSTOP1)
            IF (K.NE.KSTOP1) GO TO 345
C            THEN
              R=R+U1*DYDX(KSTOP)
  345       CONTINUE
            C(K)=Z*(R+U1*C(J1))
  315     CONTINUE
          J1=K
          U1=U2
          V1=V2
          S1=S2
          T1=T2
  305   CONTINUE
  310   CONTINUE
C
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C  BACK SUBSTITUTION
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C       IF (KSTOP-KSTRT.GT.1)
        IF (KSTOP-KSTRT.LE.1) GO TO 355
C        THEN
          DYDX(KSTOP-1)=C(KSTOP-1)
          KSTOPP=KSTOP-1
          CF(5*KSTOPP-3)=DYDX(KSTOPP)
C         IF (KSTOP-KSTRT.GT.2)
          IF (KSTOP-KSTRT.LE.2) GO TO 375
C          THEN
            KSTOP2 = KSTOP - 2
            KSTRT1 = KSTRT + 1
            DO 380 K = KSTRT1 , KSTOP2
              KDOWN = KSTRT1 + KSTOP2 - K
              DYDX(KDOWN) = C(KDOWN) - B(KDOWN) * DYDX(KDOWN+1)
              CF(5*KDOWN-3) = DYDX(KDOWN)
  380       CONTINUE
  375     CONTINUE
  355   CONTINUE
        CF(5*KSTRT-3)=DYDX(KSTRT)
C
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C COMPUTE 2ND, 3RD, 4TH ORDER COEFFICIENTS
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
        IF ( KSTRT .GT. KSTOP1) GO TO 400
        DO 395 K = KSTRT , KSTOP1
          J2=K+1
          Z=A(K)
          CF(5*K-2)= 1.5*Z*(-3.0*DYDX(K) + DYDX(J2) + Z*(-8.0*
     1    Y(J2) - 12.0*Y(K) + 20.0*H(K)))
          CF(5*K-1)= -4.0*Z*Z*(-1.5*DYDX(K) + DYDX(J2) + Z*(-7.0*
     1    Y(J2) - 8.0*Y(K) +15.0*H(K)))
          CF(5*K) = 5.0*Z*Z*Z*(0.5*(DYDX(J2)-DYDX(K)) - 3.0*Z*
     1    (Y(J2) + Y(K) - 2.0*H(K)))
  395   CONTINUE
  400   CONTINUE
      RETURN
      END
```

SUBROUTINE REPRT

```
      SUBROUTINE REPRT
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KPH(9)
      COMMON /EMIS/ NEM,EM(16),EMHC(16),EMNOX(16),ESRT(2),ESTOP,ESLP,EHS
     1LP,ENSLP,EC(80),ECHC(80),ECXN(80)
      COMMON /MIX/ MMIX,BMIX(16),STRM,STOPM,DC(45),TSTART
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /TITL/ ITTL(18)
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      COMMON /HOUR/ OZM,NGO,TM
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICZ,DIGZ,CHRZ
      COMMON /VVLBL/ FCTR,DIST,CHRSIZ,NNCHR,OZBL
      COMMON /ALOFT/FALALD(4)
      COMMON /SURFAC/FINALD(4)
      COMMON /SUNLIT/ XJ(47,10),SIGMO(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(16),XZ(16),K(16),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL,MA
     3XJ
      COMMON /MIXING/ DSTRT,DEND,AMC(5),BMC(5),CMC(5),FD(6),FG(6),
     1AMIX(16),DL,TTMAX,SRISE,SRMIN,DELH,TDIL,NMIX
      COMMON /WRTREP/PLACE(6),EMMHC(16),EMMNX(16),MEMFLG,HCB,XNXB,HINIT
      DIMENSION ITMIX(16)
      INTEGER HCSPEC,ALDSPC,PLACE
      WRITE (IOUT,315) (ITTL(I),I=1,18)
      KSTOP=JSTOP-100
      WRITE (IOUT,340) PLACE,SLA,SLO,TZ,IM,ID,IY,JSTRT,KSTOP
      NCON=SPECIE
      IF (INFO.EQ.-1) WRITE (IOUT,345) NCON
      IF(BMIX(1).GT.0.) GO TO 10
      WRITE (IOUT,350) Z1,Z2,DSTRT,DEND
      ITMIX(1)=JSTRT
      DO 6 J=2,NMIX
    6 ITMIX(J)=ITMIX(J-1)+100.
      WRITE(IOUT,530) (ITMIX(J),J=1,NMIX)
      WRITE(IOUT,535) (AMIX(J),J=1,NMIX)
      GO TO 15
   10 MMIX1=MMIX-1
      WRITE (IOUT,430) (I,I=1,MMIX1)
      WRITE (IOUT,435) (BMIX(I),I=1,MMIX)
   15 WRITE (IOUT,400)
      IF (NHC.NE.0) WRITE (IOUT,360) (HCSPEC(I),RCTY(I),I=1,NHC)
      IF (NALD.NE.0) WRITE (IOUT,360) (ALDSPC(I),ALDX(I),I=1,NALD)
      WRITE (IOUT,405) XNF(1)
      IF (NHC.EQ.0) WRITE (IOUT,390)
      IF (NALD.EQ.0) WRITE (IOUT,395)
      IF(OZIN+HCIN+XNIN.GT.0..OR.OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,445)
      IF (OZIN+HCIN+XNIN.GT.0.) WRITE (IOUT,365) OZIN,HCIN,XNIN
      IF (NI.NE.0.AND.(OZIN+HCIN+XNIN.LE.0..OR.OZAL+HCAL+XNAL.LE.0.))
     1WRITE (IOUT,445)
      IF (NI.NE.0) WRITE (IOUT,410) (REACT(I),C(I),I=1,NI)
      IF (OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,370) OZAL,HCAL,XNAL
      IEM=IABS(NEM)
      IF(MEMFLG.NE.1) GO TO 40
      WRITE(IOUT,610) HINIT,HCB,XNXB,(I,I=1,IEM)
      WRITE(IOUT,611) (EMMHC(I),I=1,IEM)
      WRITE(IOUT,612) (I,I=1,IEM)
      WRITE(IOUT,613) (EMMNX(I),I=1,IEM)
   40 CONTINUE
      IF (NEM.GT.0) WRITE (IOUT,375) (I,I=1,NEM)
      IF (NEM.GT.0) WRITE (IOUT,380) (EM(I),I=1,NEM)
      IF (NEM.LE.-1.AND.EMHC(1).GE.-3.) WRITE (IOUT,415) (I,I=1,IEM)
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.0) WRITE (IOUT,420) (EMHC(I),I=1,I
     1EM)
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,425) (I,I=1,IEM)
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,420) (EMNOX(I),I=1,
     1IEM)
  315 FORMAT (1H1,//,40X,18A4)
  340 FORMAT (1H0,//,40X,40HPHOTOLYTIC RATE CONSTANTS CALCULATED FOR,///
     1,49X,6A4,///,40X,9HLATITUDE ,F10.3,//,40X,10HLONGITUDE ,F10.3,//,4
     20X,9HTIME ZONE,F7.1,//,40X,5HDATE ,5X,3(I4,3X),//,40X,5HTIME ,7X,I
     34,3X,2HTO,3X,I4,5X,19HLOCAL DAYLIGHT TIME)
  345 FORMAT (1H0,39X,10HSOLAR NOON,I7)
  350 FORMAT (1H0,//,40X,39HDILUTION DETERMINED FROM THE FOLLOWING ,//,4
     10X,17HINVERSION HEIGHTS,5X,7HINITIAL,F7.0,5X,5HFINAL,4X,F7.0,//,40
     2X,7HTIMING ,15X,5HSTART,F9.0,5X,4HSTOP,4X,F8.0)
  360 FORMAT ((1H0,39X,8HINITIAL ,8X,3(A4,9H FRACTION,F6.3,3X)))
  365 FORMAT (/,40X,13HSURFACE LAYER,9X,5HOZONE,F8.3,6X,11HHYDROCARBON,F
     17.3,4X,3HNOX,F10.3,4H PPM)
  370 FORMAT (/,40X,5HALOFT,17X,5HOZONE,F8.3,6X,11HHYDROCARBON,F7.3,4X,3
     1HNOX,F10.3,4H PPM)
  375 FORMAT (1H0,//,40X,50HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT
     1ION OF,//,40X,54HINITIAL NON-BACKGROUND CONCENTRATION EMITTED PER
     2HOUR),//,40X,4HHOUR,3X,10I6,/,47X,7I6)
  380 FORMAT (1H0,39X,8HFRACTION,10F6.3,/,48X,7F6.3)
  390 FORMAT (1H0,39X,42HTHERE ARE NO HYDROCARBONS IN THE MECHANISM)
  395 FORMAT (1H0,39X,39HTHERE ARE NO ALDEHYDES IN THE MECHANISM)
  400 FORMAT (//)
  405 FORMAT (1H0,39X,7HNO2/NOX,6X,F6.3)
  410 FORMAT ((1H0,39X,13HSURFACE LAYER,9X,A4,1X,F8.3,6X,A4,5X,F9.3
     1,4X,A4,F9.3,4H PPM))
  415 FORMAT (1H0,//,40X,57HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT
     1ON OF INITIAL,//,40X,58HNON-BACKGROUND HYDROCARBON CONCENTRATION E
     2MITTED PER HOUR),//,45X,4HHOUR,3X,11I6,/,52X,4I6)
  420 FORMAT (1H0,44X,8HFRACTION,11F6.3,/,53X,4F6.3,/,53X,F6.3)
  425 FORMAT (1H0,//,40X,58HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT
     1ION OF INITIAL,//,40X,50HNON-BACKGROUND NOX CONCENTRATION EMITTED
     2PER HOUR),//,45X,4HHOUR,3X,11I6,/,52X,4I6)
  430 FORMAT (1H0,//,40X,39HDILUTION DETERMINED FROM THE FOLLOWING ,//,4
     10X,46HMIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR),//,40X,4HHOUR
     2,9X,1H0,9I8,/,46X,6I8)
  435 FORMAT (1H0,39X,8HHEIGHT   ,10F8.1,/,48X,6F8.1)
  445 FORMAT (1H0,//,40X,26HTRANSPORTED CONCENTRATIONS )
  530 FORMAT(1H0,//40X,46HMIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
     1,//,40X,4HTIME,3X,10I7/47X,6I7)
  535 FORMAT(1H0,39X,6HHEIGHT,2X,10F7.1/48X,6F7.1)
  610 FORMAT(1H0,//,40X,46HEMISSION FRACTIONS COMPUTED FROM THE FOLLOWIN
     1G//42X,32HINITIAL MIXING HEIGHT (METERS) :,2X,F6.1//42X,
     233HINITIAL HC CONCENTRATION (PPMC) :,2X,F5.2//42X,
     333HINITIAL NOX CONCENTRATION (PPM) :,2X,F5.3//42X,
     436HHOURLY EMISSION DENSITIES (KG/KM2) :,//45X,
     54HHOUR,2X,10(I5,3X)/51X,5(I5,3X))
  611 FORMAT(1H0,44X,4HHC  ,10F8.1/49X,5F8.1)
  612 FORMAT(1H0,44X,4HHOUR,2X,10(I5,3X)/51X,5(I5,3X))
  613 FORMAT(1H0,44X,4HNOX ,10F8.1/49X,5F8.1)
      END
```

SUBROUTINE MCHSET

```
      SUBROUTINE MCHSET (NX,NY)
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TFRNT,TSTEP
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /MCH1/ IPS(200,7)
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KPH(9)
      DIMENSION KRS(7)
      DATA IBLANK/'    '/
      IF (NY.NE.1) GO TO 10
      NS=1
      NR=0
      DO 5 I=1,200
      A(I)=0.
      S(I)=0.
      R(I)=0.
      DO 5 J=1,7
      IRS(I,J)=IBLANK
    5 KR(I,J)=0
   10 NS=NS-1
      WRITE (IOUT,40)
   15 READ(IN,30) (KPS(I),I=1,3),J,JJ,(KRS(LL),LL=4,7),RTE,ENERGY
      IF (JJ.GT.0) J=JJ*100+J
      DO 16 II=1,7
   16 IRS(J,II)=KRS(II)
      A(J)=RTE
      S(J)=ENERGY
      WRITE (IOUT,35) J,(IRS(J,K),K=1,7),A(J),S(J)
      KR(J,1)=100
      IF (IP.EQ.0) GO TO 25
      DO 20 I=1,IP
      IF (J.NE.IPH(I)) GO TO 20
      RFCT(I)=A(J)
      GO TO 25
   20 CONTINUE
   25 IF (J.GT.NR) NR=J
      IF (J.NE.NX) GO TO 15
      CALL MATRX
      RETURN
C
   30 FORMAT (2(A4,2X),A4,I2,5X,I1,A4,3(4X,A4),2X,F10.2,1X,F7.2)
   35 FORMAT (1H0,I10,10X,3A10,2H= ,4X,4A10,1P2E15.3)
   40 FORMAT (1H1,5X,18HTHE REACTIONS ARE /)
      END
      SUBROUTINE MATRX
      COMMON /CALC/ NR,IR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /MCH1/ KR(200,7)
      INTEGER SPECIS
      DATA IBLANK/4H    /,MBLANK/4HM   /
      NOLD=NS+1
      DO 90 I=1,NR
      IF (IR(I,2).EQ.NOLD.OR.IR(I,3).EQ.NOLD) IR(I,3)=99
      IF (IR(I,2).EQ.NOLD) IR(I,2)=0
      IF (IR(I,1).EQ.NOLD) IR(I,1)=99
      IF (IR(I,1).EQ.NOLD) IR(I,3)=99
      IF (IABS(IR(I,1)).NE.100) GO TO 90
      IF (KR(I,1).NE.IBLANK) GO TO 5
      IF (KR(I,3).NE.IBLANK) KR(I,1)=KR(I,3)
      KR(I,3)=IBLANK
      IF (KR(I,1).NE.IBLANK) GO TO 5
      KR(I,1)=KR(I,2)
      KR(I,2)=IBLANK
    5 IF (KR(I,2).NE.IBLANK) GO TO 10
      IF (KR(I,3).NE.IBLANK) KR(I,2)=KR(I,3)
      KR(I,3)=IBLANK
   10 DO 15 K=4,7
      IF (KR(I,K).EQ.MBLANK) KR(I,K)=IBLANK
   15 CONTINUE
      IF (KR(I,4).NE.IBLANK) GO TO 30
      DO 20 K=1,3
      INDEX=8-K
      IF (KR(I,INDEX).NE.IBLANK) GO TO 25
   20 CONTINUE
      INDEX=5
   25 KR(I,4)=KR(I,INDEX)
      KR(I,INDEX)=IBLANK
      IF (KR(I,1).NE.IBLANK.OR.KR(I,4).NE.IBLANK) GO TO 30
      IR(I,1)=0
      GO TO 90
   30 CONTINUE
      IF (KR(I,5).NE.IBLANK) GO TO 35
      IF (KR(I,7).NE.IBLANK) KR(I,5)=KR(I,7)
      KR(I,7)=IBLANK
      IF (KR(I,5).NE.IBLANK) GO TO 35
      KR(I,5)=KR(I,6)
      KR(I,6)=IBLANK
   35 K=KR(I,6)
      IF (K.NE.IBLANK) GO TO 40
      KR(I,6)=KR(I,7)
      KR(I,7)=K
   40 DO 85 J=1,7
      K=KR(I,J)
      IF (J.GT.3) GO TO 65
      IF (K.NE.MBLANK) GO TO 60
      GO TO (45,50,55),J
   45 KR(I,1)=KR(I,2)
   50 KR(I,2)=KR(I,3)
      KR(I,3)=MBLANK
   55 IR(I,3)=99
   60 K=KR(I,J)
      IF (KR(I,1).EQ.IBLANK) IR(I,1)=99
      IF (KR(I,1).EQ.IBLANK) K=99
      IF (J.EQ.3.AND.K.EQ.MBLANK) K=99
   65 IF (K.EQ.MBLANK.OR.K.EQ.IBLANK) IR(I,J)=0
      IF (K.EQ.IBLANK.OR.K.EQ.99) GO TO 85
      IF (NS.NE.0) GO TO 70
      NS=1
      GO TO 80
   70 DO 75 L=1,NS
      IF (K.NE.SPECIS(L)) GO TO 75
      IR(I,J)=L                                                         AM  71
      GO TO 85                                                          AM  72
   75 CONTINUE                                                          AM  73
      IF (SPECIS(NS).NE.MBLANK) NS=NS+1                                 AM  74
   80 SPECIS(NS)=K                                                      AM  75
      C(NS+1)=C(NS)                                                     AM  76
      C(NS)=0.                                                          AM  77
      IR(I,J)=NS                                                        AM  78
   85 CONTINUE                                                          AM  79
   90 CONTINUE                                                          AM  80
      IF (SPECIS(NS).NE.MBLANK) NS=NS+1                                 AM  81
      SPECIS(NS)=MBLANK                                                 AM  82
      RETURN                                                            AM  83
      END                                                               AM  84-
```

SUBROUTINE RATES

```
      SUBROUTINE RATES (C,N)
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSFC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FEX(2),CR(81),REACT(81),NI,PLSP
      DIMENSION C(N)
      DIMENSION SIG(81)
      INTEGER SPECIS,REACT
      FCT=(1./298.)-(1./TEMP)
      DO 5 I=1,81
    5 SIG(I)=0.
      IF (N.LE.0) GO TO 20
      DO 15 I=1,N
      DO 10 J=1,NS
      IF (SPECIS(J).EQ.REACT(I)) SIG(J)=C(I)
      IF (SPECIS(J).EQ.REACT(I)) GO TO 15
   10 CONTINUE
      SIG(NS+1)=SIG(NS+1)+C(I)
   15 CONTINUE
   20 N=NS
      M=N-1
      C(N)=0.
      DO 25 I=1,M
      C(N)=C(N)+SIG(I)
   25 C(I)=SIG(I)
      BK=0.
      C(N)=C(N)+SIG(NS+1)
      IF (SIG(N).NE.0.) BK=SIG(N)-C(N)
      IF (SIG(N).NE.0.) C(N)=SIG(N)
      NP=0
      DO 35 I=1,NR
      IF (KR(I,1).EQ.0) GO TO 35
      ITYPE(I)=2
      IF (KR(I,1).EQ.99.AND.KR(I,3).EQ.99) KR(I,1)=N
      IF (KR(I,1).EQ.N.AND.KR(I,3).EQ.99) KR(I,3)=0
      IF (KR(I,2).EQ.0.AND.KR(I,3).EQ.99) KR(I,2)=N
      IF (KR(I,2).EQ.N.AND.KR(I,3).EQ.99) KR(I,3)=0
      IF (KR(I,2).EQ.0) ITYPE(I)=1
      IF (KR(I,3).NE.0) ITYPE(I)=3
      IF (KR(I,3).EQ.99) KR(I,3)=N
      DO 30 J=4,7
      IF (KR(I,J).LT.0) KR(I,J)=-KR(I,J)
   30 CONTINUE
      IF (ABS(S(I)).EQ.0.) R(I)=A(I)
      IF (ABS(S(I)).NE.0.) R(I)=A(I)*EXP(S(I)*FCT)
   35 CONTINUE
      RETURN
      END
```

SUBROUTINE SPARS

```
      SUBROUTINE SPARS (IA,JA,N)
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IB(80),
     1JB(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN,XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      DIMENSION IA(N), JA(N)
      DO 5 I=1,N
    5 IA(I)=1
      KT=0
      IA(N+1)=1
      JA(1)=0
      DO 70 IR=1,NR
      IF (KR(IR,1).EQ.0.OR.KR(IR,1).EQ.99) GO TO 70
      MT=ITYPE(IR)
      DO 65 K=1,MT
      I=KR(IR,K)
      DO 30 L=1,MT
      J=KR(IR,L)
      K1=IA(J)
      K2=IA(J+1)-1
      IF (K1.GT.K2) GO TO 15
      DO 10 M=K1,K2
      IF (I.EQ.JA(M)) GO TO 30
   10 CONTINUE
   15 DO 20 M=J,N
   20 IA(M+1)=IA(M+1)+1
      KT=KT+1
      KD=KT-K2
      K2=K2+1
      DO 25 M=1,KD
   25 JA(KT+2-M)=JA(KT+1-M)
      JA(K2)=I
   30 CONTINUE
      K1=IA(I)
      DO 60 L=4,7
      K2=IA(I+1)-1
      J=KR(IR,L)
      IF (J) 60,65,35
   35 IF (K1.GT.K2) GO TO 45
      DO 40 M=K1,K2
      IF (J.EQ.JA(M)) GO TO 60
   40 CONTINUE
   45 DO 50 M=I,N
   50 IA(M+1)=IA(M+1)+1
      KT=KT+1
      KD=KT-K2
      K2=K2+1
      DO 55 M=1,KD
   55 JA(KT+2-M)=JA(KT+1-M)
      JA(K2)=J
   60 CONTINUE
   65 CONTINUE
   70 CONTINUE
      DO 80 I=1,N
      K1=IA(I)+1
      K2=IA(I+1)-1
      IF (K1.GT.K2) GO TO 80
      MT=K2-K1+1
      DO 75 K=1,MT
      DO 75 M=K1,K2
      IF (JA(M).GT.JA(M-1)) GO TO 75
      J=JA(M-1)
      JA(M-1)=JA(M)
      JA(M)=J
   75 CONTINUE
   80 CONTINUE
      M=N
      DO 200 I=1,M
      IF(IA(I+1).GT.IA(I)) GO TO 200
      NM=I+1
      NN=N+1
      KMIN=IA(NM)
      KMAX=IA(NN)
      DO 210 J=KMIN,KMAX
      KM=KMAX+KMIN-J
  210 JA(KM)=JA(KM-1)
      KNOW=IA(I)
      JA(KNOW)=I
      DO 220 LL=NM,NN
  220 IA(LL)=IA(LL)+1
  200 CONTINUE
      RETURN
      END
```

SUBROUTINE SORDER

```
      SUBROUTINE SORDER (N,IA,JA,P,Q,MAX,V,L,IER)
      INTEGER IA(1),JA(1),P(1),Q(1),V(1),L(1)
      INTEGER S,SFS,PI,PJ,VI,VJ,VK,QVK,DTHR,DMIN
      IER=0
      DO 5 S=1,MAX
    5 L(S)=S+1
      SFS=1
      L(MAX)=0
      DO 10 K=1,N
      P(K)=K
      Q(K)=K
      V(K)=1
   10 L(K)=0
      SFS=SFS+N
      DO 50 K=1,N
      JMIN=IA(K)
      JMAX=IA(K+1)-1
      IF(JMIN.GT.JMAX+1) GO TO 145
      KDIAG=0
      DO 45 J=JMIN,JMAX
      VJ=JA(J)
      IF (VJ.NE.K) GO TO 15
      KDIAG=1
      GO TO 45
   15 LLK=K
   20 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 25
      IF (V(LLK)-VJ) 20,30,25
   25 LLK=SFS
      IF (LLK.EQ.0) GO TO 150
      SFS=L(SFS)
      V(K)=V(K)+1
      V(LLK)=VJ
      L(LLK)=L(LK)
      L(LK)=LLK
   30 LLK=VJ
   35 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 40
      IF (V(LLK)-K) 35,45,40
   40 LLK=SFS
      IF (LLK.EQ.0) GO TO 150
      SFS=L(SFS)
      V(VJ)=V(VJ)+1
      V(LLK)=K
      L(LLK)=L(LK)
      L(LK)=LLK
   45 CONTINUE
      IF (KDIAG.EQ.0) GO TO 160
   50 CONTINUE
      J=0
      DTHR=0
      DMIN=N
      I=0
   55 I=I+1
      IF (I.GT.N) GO TO 140
      JMIN=MAX0(J+1,I)
      IF (JMIN.GT.N) GO TO 70
   60 DO 65 J=JMIN,N
      VI=P(J)
      IF (V(VI).LE.DTHR) GO TO 75
      IF (V(VI).LT.DMIN) DMIN=V(VI)
   65 CONTINUE
   70 DTHR=DMIN
      DMIN=N
      JMIN=I
      GO TO 60
   75 PJ=P(I)
      P(J)=PJ
      Q(PJ)=J
      PI=VI
      P(I)=PI
      Q(PI)=I
      LI=VI
   80 LI=L(LI)
      IF (LI.EQ.0) GO TO 105
      VK=V(LI)
      LLK=VK
      LJ=VI
   85 LJ=L(LJ)
      IF (LJ.EQ.0) GO TO 100
      VJ=V(LJ)
      IF (VJ.EQ.VK) GO TO 85
   90 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 95
      IF (V(LLK)-VJ) 90,85,95
   95 LLK=SFS
      IF (LLK.EQ.0) GO TO 155
      SFS=L(SFS)
      V(VK)=V(VK)+1
      V(LLK)=VJ
      L(LLK)=L(LK)
      L(LK)=LLK
      GO TO 85
  100 IF (V(VK).GT.V(VI)) GO TO 80
      I=I+1
      QVK=Q(VK)
      PI=P(I)
      P(QVK)=PI
      Q(PI)=QVK
      P(I)=VK
      Q(VK)=I
      GO TO 80
  105 LI=VI
  110 IF (L(LI).EQ.0) GO TO 135
      LI=L(LI)
      VK=V(LI)
      LLK=VK
      QVK=MIN0(Q(VK),I)
  115 LK=LLK
      LLK=L(LK)
      IF (LLK.EQ.0) GO TO 120
      VJ=V(LLK)
      IF (Q(VJ).GT.QVK) GO TO 115
      V(VK)=V(VK)-1
      L(LK)=L(LLK)
      L(LLK)=SFS
      SFS=LLK
      LLK=LK
      GO TO 115
  120 IF (Q(VK).LE.I) GO TO 130
      IF (V(VK).LE.DTHR) GO TO 125
      IF ((DTHR.LT.V(VK)).AND.(V(VK).LT.DMIN)) DMIN=V(VK)
      GO TO 110
  125 J=MIN0(Q(VK)-1,J)
      DTHR=V(VK)
      GO TO 110
  130 L(LK)=SFS
      SFS=L(VK)
      GO TO 110
  135 L(LI)=SFS
      SFS=L(VI)
      GO TO 55
  140 RETURN
  145 CALL YSMER (3HROW,K,13H OF A IS NULL)
      GO TO 165
  150 CALL YSMER (3HROW,K,16H EXCEEDS STORAGE)
      GO TO 165
```

```
155 CALL YSMER (6HVERTEX,VI,16H EXCEEDS STORAGE)
    GO TO 165
160 CALL YSMER (6HCOLUMN,K,19H.. DIAGONAL MISSING)
165 IER=1
    RETURN
    END
```

SUBROUTINE NSCORD

```
      SUBROUTINE NSCORD (N,IA,JA,IAWORK,JAWORK,C,IR,ICT)
      INTEGER IA(1),JA(1),IAWORK(1),JAWORK(1),C(1),IR(1),ICT(1)
      DO 5 I=1,N
    5 ICT(I)=0
      IAWORK(1)=1
      DO 15 K=1,N
      ICK=C(K)
      JMIN=IAWORK(K)
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1
      IAWORK(K+1)=JMAX+1
      IF (JMIN.GT.JMAX) GO TO 15
      IAINK=IA(ICK)-1
      DO 10 J=JMIN,JMAX
      IAINK=IAINK+1
      JAOUTJ=JA(IAINK)
      JAOUTJ=IR(JAOUTJ)
      JAWORK(J)=JAOUTJ
   10 ICT(JAOUTJ)=ICT(JAOUTJ)+1
   15 CONTINUE
      IA(1)=1
      DO 20 I=1,N
      IA(I+1)=IA(I)+ICT(I)
   20 ICT(I)=IA(I)
      DO 30 I=1,N
      JMIN=IAWORK(I)
      JMAX=IAWORK(I+1)-1
      IF (JMIN.GT.JMAX) GO TO 30
      DO 25 J=JMIN,JMAX
      JAOUTJ=JAWORK(J)
      ICTJ=ICT(JAOUTJ)
      JA(ICTJ)=I
   25 ICT(JAOUTJ)=ICTJ+1
   30 CONTINUE
      RETURN
      END
```

SUBROUTINE NSSFAC

```
      SUBROUTINE NSSFAC (N,IA,JA,MAXPL,IL,JL,ISL,MAXPU,IU,JU,ISU
     1,IRL,JRL,IER)
      INTEGER IA(1),JA(1),IRA(80),JRA(80),IL(1),JL(1),ISL(1)
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1),IRU(80),JRU(80)
      INTEGER P(80),V(80),IRAC(80)
      INTEGER VI,VJ,PK,PPK,PI,CEND,REND
      IER=0
      DO 5 K=1,N
      IRAC(K)=0
      JRA(K)=0
      JRL(K)=0
    5 JRU(K)=0
      DO 10 K=1,N
      IAK=IA(K)
      IF(IAK.GT.IA(K+1)) GO TO 210
      IF (JA(IAK).GT.K) GO TO 10
      JAIAK=JA(IAK)
      JRA(K)=IRAC(JAIAK)
      IRAC(JAIAK)=K
   10 IRA(K)=IAK
      JLPTR=0
      IL(1)=1
      JUPTR=0
      IU(1)=1
      DO 205 K=1,N
      P(1)=1
      V(1)=N+1
      LSFS=2
      VJ=IRAC(K)
      IF (VJ.EQ.0) GO TO 30
   15 PPK=1
   20 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 20,230,25
   25 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
      LSFS=LSFS+1
      VJ=JRA(VJ)
      IF (VJ.NE.0) GO TO 15
   30 LASTI=0
      I=K
   35 I=JRU(I)
      IF (I.EQ.0) GO TO 60
      PPK=1
      JMIN=IRL(I)
      JMAX=ISL(I)+IL(I+1)-IL(I)-1
      IF (LASTI.GT.I) GO TO 40
      LASTI=I
      LASTID=JMAX-JMIN
      IF (JL(JMIN).NE.K) LASTID=LASTID+1
   40 IF (JMIN.GT.JMAX) GO TO 35
      DO 55 J=JMIN,JMAX
      VJ=JL(J)
   45 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 45,55,50
   50 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
      PPK=LSFS
      LSFS=LSFS+1
   55 CONTINUE
      GO TO 35
   60 PI=P(1)
      IF (V(PI).NE.K) GO TO 235
      IF (LASTI.EQ.0) GO TO 65
      IF (LASTID.NE.LSFS-3) GO TO 65
      IRLL=IRL(LASTI)
      ISL(K)=IRLL+1
      IF (JL(IRLL).NE.K) ISL(K)=ISL(K)-1
      IL(K+1)=IL(K)+LASTID
      IRL(K)=ISL(K)
      GO TO 85
   65 ISL(K)=JLPTR+1
      PI=P(1)
      PI=P(PI)
      VI=V(PI)
   70 IF (VI.GT.N) GO TO 80
      JLPTR=JLPTR+1
      IF (JLPTR.GT.MAXPL) GO TO 240
      JL(JLPTR)=VI
      PI=P(PI)
      VI=V(PI)
      GO TO 70
   80 IRL(K)=ISL(K)
      IL(K+1)=IL(K)+JLPTR-ISL(K)+1
   85 P(1)=1
      V(1)=N+1
      LSFS=2
      JMIN=IRA(K)
      JMAX=IA(K+1)-1
      IF (JMIN.GT.JMAX) GO TO 105
      DO 100 J=JMIN,JMAX
      VJ=JA(J)
      PPK=1
   90 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 90,215,95
   95 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
  100 LSFS=LSFS+1
  105 LASTI=0
      I=K
  110 I=JRL(I)
      IF (I.EQ.0) GO TO 135
      PPK=1
      JMIN=IRU(I)
      JMAX=ISU(I)+IU(I+1)-IU(I)-1
      IF (LASTI.GT.I) GO TO 115
      LASTI=I
      LASTID=JMAX-JMIN
      IF (JU(JMIN).NE.K) LASTID=LASTID+1
  115 IF (JMIN.GT.JMAX) GO TO 110
      DO 130 J=JMIN,JMAX
      VJ=JU(J)
  120 PK=PPK
      PPK=P(PK)
      IF (V(PPK)-VJ) 120,130,125
  125 P(PK)=LSFS
      V(LSFS)=VJ
      P(LSFS)=PPK
      PPK=LSFS
  130 LSFS=LSFS+1
      GO TO 110
  135 PI=P(1)
      IF (V(PI).NE.K) GO TO 220
      IF (LASTI.EQ.0) GO TO 140
      IF (LASTID.NE.LSFS-3) GO TO 140
      IRUL=IRU(LASTI)
      ISU(K)=IRUL+1
      IF (JU(IRUL).NE.K) ISU(K)=ISU(K)-1
      IU(K+1)=IU(K)+LASTID
      IRU(K)=ISU(K)
      GO TO 160
  140 ISU(K)=JUPTR+1
      PI=P(1)
      PI=P(PI)
      VI=V(PI)
```

```
145 IF (VI.GT.N) GO TO 155
    JUPTR=JUPTR+1
    IF (JUPTR.GT.MAXPU) GO TO 225
    JU(JUPTR)=VI
    PI=P(PI)
    VI=V(PI)
    GO TO 145
155 IRU(K)=ISU(K)
    IU(K+1)=IU(K)+JUPTR-ISU(K)+1
160 I=K
165 I1=JRL(I)
    CEND=ISL(I)+IL(I+1)-IL(I)
    IF (IRL(I).GE.CEND) GO TO 170
    IRLI=IRL(I)
    J=JL(IRLI)
    JRL(I)=JRL(J)
    JRL(J)=I
170 I=I1
    IF (I.EQ.0) GO TO 175
    IRL(I)=IRL(I)+1
    GO TO 165
175 I=K
180 I1=JRU(I)
    REND=ISU(I)+IU(I+1)-IU(I)
    IF (IRU(I).GE.REND) GO TO 185
    IRUI=IRU(I)
    J=JU(IRUI)
    JRU(I)=JRU(J)
    JRU(J)=I
185 I=I1
    IF (I.EQ.0) GO TO 190
    IRU(I)=IRU(I)+1
    GO TO 180
190 I=IRAC(K)
    IF (I.EQ.0) GO TO 205
195 I1=JRA(I)
    IRA(I)=IRA(I)+1
    IF (IRA(I).GE.IA(I+1)) GO TO 200
    IRAI=IRA(I)
    IF (JA(IRAI).GT.I) GO TO 200
    JAIRAI=JA(IRAI)
    JRA(I)=IRAC(JAIRAI)
    IRAC(JAIRAI)=I
200 I=I1
    IF (I.NE.0) GO TO 195
205 CONTINUE
    ISL(N)=JLPTR
    ISU(N)=JUPTR
    RETURN
210 CALL YSMER (3HROW,K,13H OF A IS NULL)
    GO TO 245
215 CALL YSMER (3HROW,K,20H HAS DUPLICATE ENTRY)
    GO TO 245
220 CALL YSMER (3HROW,K,17H HAS A NULL PIVOT)
    GO TO 245
225 CALL YSMER (3HROW,K,19H EXCEEDS JU STORAGE)
    GO TO 245
230 CALL YSMER (3HCOL,K,20H HAS DUPLICATE ENTRY)
    GO TO 245
235 CALL YSMER (3HCOL,K,17H HAS A NULL PIVOT)
    GO TO 245
240 CALL YSMER (3HCOL,K,19H EXCEEDS JL STORAGE)
245 IER=1
    RETURN
    END
```

SUBROUTINE VVLBLF

```
      SUBROUTINE VVLBLF (X2,Y2)
C
C     *** SETS A LINE LABEL INTO A VECTOR PLOT PROVIDING THAT
C         A CALL TO SUBROUTINE PLTLBL HAS PRESET THE NECESSARY
C         PARAMETERS IN /VVLBL/
C             GW LUNDBERG/SAI  DEC 1977
C
C     X2,Y2     THE TERMINAL POINT OF THE CURRENT VECTOR
C               IN INCHES FROM PRESENT PLOT ORIGIN
C
C     *** NOTES --
C         (1) THERE ARE THREE ENTRY POINTS -- VVLBLF SETS UP THE
C             PARAMETERS FOR VVLBLC WHICH ACTUALLY DOES THE LABELING.
C             VVLBLL CLEANS UP IN CASE THERE WAS NOT ENOUGH
C             ROOM FOR THE LAST LABEL
C         (2) THE LABELS ARE SEPERATED BY DIST INCHES EXCEPT FOR
C             THE FIRST LABEL WHICH STARTS FACT*DIST INCHES FROM
C             THE BEGINNING OF THE VECTOR PLOT -- THIS PROVIDES FOR
C             STAGGERED LABELS.
C
      DIMENSION XSV(20), YSV(20)
C
C     *** DIST IS THE DISTANCE IN INCHES BETWEEN LABELS.  FACT
C         IS THE FACTOR (0-1) OF DIST TO USE FOR THE FIRST LABEL.
C         CHRSZ IS THE SIZE OF THE LABEL CHARACTERS IN INCHES.
C         NCHR IS THE NUMBER OF CHARACTERS (0-10), AND LABEL
C         IS THE A-FORMATED TEXT OF THE LABEL
      COMMON /VVLBL/ FACT,DIST,CHRSZ,NCHR,OZL
      DATA MXSV/20/
C
C     *** MOVE THE PEN TO THE FIRST POINT
      CALL PLOT (X2,Y2,3)
C
C     *** IF THERE ARE TO BE NO LABELS -- JUST RETURN
      IF (NCHR.EQ.0) RETURN
C
C     *** SET UP THE OFFSET NECESSARY TO CENTER THE LABEL AND
C         THE DISTANCE REQUIRED BY THE LABEL
      OFF=CHRSZ/2.
      SZLBL=NCHR*CHRSZ+2.*OFF-0.3*CHRSZ
C
C     *** INITALIZE THE ACCUMULATED LENGTH OF THE VECTORS, THE
C         LENGTH REQUIRED BEFORE FIRST LABEL, AND THE NUMBER
C         OF SAVED POINTS (VECTORS) THAT MAY HAVE BEEN PREEMPTED
C         BY THE LABEL
      TOTSZ=0.
      SKPSZ=FACT*DIST
      NSV=0
C
C     *** REMEMBER THE STARTING LOCATION OF FIRST VECTOR
      X1=X2
      Y1=Y2
C
      RETURN
C
C***********************************************************
C                   ENTRY VVLBLC
C***********************************************************
C
      ENTRY VVLBLC (X2,Y2)
C
C     *** IF THERE ARE TO BE NO LABELS -- PLOT THE VECTOR AND RETURN
      IF (NCHR.GT.0) GO TO 5
      CALL PLOT (X2,Y2,2)
      RETURN
C
C     *** IF SEEKING ROOM FOR THE LABEL -- SKIP FOLLOWING
    5 IF (NSV.GT.0) GO TO 15
C
C     *** CALCULATE THIS VECTOR LENGTH AND ADD TO THE ACCUMULATED
```

```
C         LENGTH.  IF A LABEL IS TO START IN THIS VECTOR, SKIP TO
C         120, ELSE PLOT THE VECTOR AND RETURN
      VECSZ=SQRT((X2-X1)**2+(Y2-Y1)**2)
      TOTSZ=TOTSZ+VECSZ
      IF (TOTSZ.GT.SKPSZ) GO TO 10
      CALL PLOT (X2,Y2,2)
      X1=X2
      Y1=Y2
      RETURN
C
C     *** ITS TIME FOR A LABEL -- LOCATE START
   10 RATIO=(VECSZ-TOTSZ+SKPSZ)/VECSZ
      X1L=X1+RATIO*(X2-X1)
      Y1L=Y1+RATIO*(Y2-Y1)
C
C     *** PLOT SUBVECTOR AND REMEMBER THE END POINT
      CALL PLOT (X1L,Y1L,2)
      X1=X1L
      Y1=Y1L
C
C     *** FIND OUT IF THERE IS ENOUGH ROOM LEFT IN THIS VECTOR
C         FOR THE LABEL -- IF THERE ISNT, SAVE (X2,Y2) AND RETURN
   15 HAVSZ=SQRT((X2-X1L)**2+(Y2-Y1L)**2)
      IF (HAVSZ.GE.SZLBL) GO TO 20
      NSV=NSV+1
C
C     *** CHECK FOR OVERFLOW
      IF (NSV.GT.MXSV) STOP
      XSV(NSV)=X2
      YSV(NSV)=Y2
      X1=X2
      Y1=Y2
      RETURN
C
C     *** CALCULATE THE END OF THE LABEL
C         IM SURE THERE IS AN EASIER WAY TO DO THIS, BUT IT
C         ESCAPES ME
   20 A=(X2-X1)**2+(Y2-Y1)**2
      B=-2*((X1L-X1)*(X2-X1)+(Y1L-Y1)*(Y2-Y1))
      C=(X1L-X1)**2+(Y1L-Y1)**2-SZLBL*SZLBL
C
      SQRTD=SQRT(B*B-4*A*C)
      T1=(-B+SQRTD)/(2*A)
      T2=(-B-SQRTD)/(2*A)
C
C     *** PICK THE MINIMUM T BETWEEN 0-1 (MUST BE ONE)
      IF (T1.LT.0.) T1=1.
      IF (T2.LT.0.) T2=1.
      RATIO=AMIN1(T1,T2)
C
C     *** SET LABEL END POINT
      X2L=X1+RATIO*(X2-X1)
      Y2L=Y1+RATIO*(Y2-Y1)
C
C     *** CALCULATE LABEL ANGLE
      DX=X2L-X1L
      DY=Y2L-Y1L
      ANG=0.
      IF (DY.NE.0.) ANG=ATAN2(DY,DX)
C
      XL=X1L
      YL=Y1L
      COSA=COS(ANG)
      SINA=SIN(ANG)
C
C     *** REVERSE EVERYTHING IF ANGLE IN QUADRANTS 2 OR 3
      IF (DX.GE.0.) GO TO 25
      XL=X2L
      YL=Y2L
      COSA=-COSA
      SINA=-SINA
      IF (DY.GE.0.) ANG=ANG-3.1415926536
      IF (DY.LT.0.) ANG=ANG+3.1415926536
   25 ANGD=ANG*180./3.1415926536
C
C     *** LOCATE AND PLOT LABEL
      XL=XL+OFF*COSA+OFF*SINA
      YL=YL+OFF*SINA-OFF*COSA
      IDG=NCHR-2
      CALL NUMBER (XL,YL,CHRSZ,OZL,ANGD,IDG)
C
C     *** FINISH OFF THIS SEQMENT BY MEANS OF A PSUEDO REENTRY
      TOTSZ=0.
      SKPSZ=DIST
      NSV=0
      X1=X2L
      Y1=Y2L
      CALL PLOT (X1,Y1,3)
      GO TO 5
C
C*****************************************************************
C                   ENTRY VVLBLL
C*****************************************************************
C
      ENTRY VVLBLL (X2,Y2)
C
C     *** PLOT THE SAVED VECTORS IF ANY
      IF (NSV.EQ.0) RETURN
      DO 30 I=1,NSV
      CALL PLOT (XSV(I),YSV(I),2)
   30 CONTINUE
      NSV=0
      RETURN
C
      END
```

SUBROUTINE MIXSET

```
      SUBROUTINE MIXSET
      COMMON /MIX/ NMIX,AMIX(16),STRM,STOPM,DC(45),TSTART
      STRM=0.
      STOPM=FLOAT(NMIX-1)*60.
      NMX4=(NMIX-1)*3
      DO 5 I=1,NMX4
    5 DC(I)=0.
      NMIX1=NMIX-1
      DO 10 I=1,NMIX1
      K=3*I-2
      DC(K)=(AMIX(I+1)-AMIX(I))/60.
   10 CONTINUE
      RETURN
      END
```

SUBROUTINE NEWLIN

```
      SUBROUTINE NEWLIN (N,OT,HCT,SX,NS,NE,NL,NR,XNL,NPL,TOL,NUL,NTL,II)
      COMMON /NEED/ HC,XN,NN,NB,R(20),OZP(20),OZN(8,20),RHO(8,20),M,OC(4
     1 ),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      DIMENSION XNL(20), OT(20), HCT(20), YP(20), TM(20), NUL(20), NTL(2
     10)
      IT=1
      ISAV=0
      IF (OT(N-1).LT.TOL*OT(N)) GO TO 10
      IF (N.LE.2) GO TO 10
      DO 5 I=NS,NE
      J=NE-I+NS
      IF (OZP(J).LE.OT(N).AND.OZP(J).GE.OT(N-1)) GO TO 10
    5 CONTINUE
      N=N-1
   10 CALL CURV1 (N,OT,HCT,SP1,SP2,YP,TM,SX)
      IF (NL.LT.6) GO TO 12
      IF (IT.GT.0) GO TO 12
      DO 11 I=NS,NE
      NUL(I)=0
      NTL(I)=0
   11 CONTINUE
      IT=1
   12 DO 20 I=NS,NE
      IF (OZP(I).GT.OT(N)) GO TO 25
      IF (OZP(I).LT.OT(1).AND.NL.EQ.6) GO TO 20
      IF (OZP(I).LT.OT(1).AND.NL.GT.6) GO TO 25
      IF (NL.LT.6) GO TO 15
      IF (IT.GT.0) NUL(I)=NUL(I)+1
      IF (NUL(I).EQ.1) NTL(I)=II
      IF (NUL(I).EQ.1) NUL(I)=II
   15 XNL(I-NR)=CURV2(OZP(I),N,OT,HCT,YP,SX,IT)
      IF (IT.GT.0) GO TO 20
      ISAV=I
      SX=SX*10.
      SX=AMAX1(-50.,SX)
      GO TO 10
   20 IT=2
      I=NE+1
   25 NPL=I-1
      RETURN
      END
      BLOCK DATA
      COMMON /CALC/ NR,KR(200,7),A(200),S(200),R(200),ITYPE(200),IA(80),
     1JA(2500),DILUT,TEMP,ERR,START,STOPP,SPECIS(81),TPRNT,TSTEP
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FL
     1ST,TLST,NSPARS
      COMMON /SPEC/ NS,HCSPEC(10),CARB(10),RCTY(10),ALDSPC(4),ALDX(4),XN
     1F(2),IH(10),INOX(2),IALD(4),FINHC(10),FALHC(10),NHC,NALD,OZIN,OZAL
     2,HCIN,HCAL,XNIN.XNAL,KOZ,ALDCRB(4),FENX(2),C(81),REACT(81),NI,PLSP
      COMMON /PHOTON/ CF(45,8),P(16,9),IPH(9),IP,RFCT(9),KFACT,KFH(9)
      COMMON /EMIS/ NEM,EM(16),EMHC(16),EMNOX(16),ESRT(2),ESTOP,ESLP,EHS
     1LP,ENSLP,EC(80),ECHC(80),ECXN(80)
      COMMON /MIX/ MMIX,BMIX(16),STRM,STOPM,DC(45),TSTART
      COMMON /INOUT/ IN,IOUT,ITAPE
      COMMON /TITL/ ITTL(18)
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),MR
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8),XNLL(8)
      COMMON /HCUR/ OZM,NGO,TM
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T
     1ICZ,DIGZ,CHRZ
      COMMON /VVLBL/ FCTR,DIST,CHRSIZ,NNCHR,OZBL
      COMMON /ALOFT/FALALD(4)
      COMMON /SURFAC/FINALD(4)
      COMMON /SUNLIT/ XJ(47,10),SIGMO(31,10),PHI(31,10),Z(10),RTCON(10),
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI
     2ME(16),XZ(16),K(16),JSTRT,JSTOP,PSPEC(11),MNLM(11),MXLM(11),MAXL,
     3MAXJ
      COMMON /WRTREP/PLACE(6),EMMHC(16),EMMNX(16),MEMFLG,HCB,XNXB,HINIT
      COMMON /MIXING/ DSTRT,DEND.AMC(5),BMC(5),CMC(5),FD(6),FG(6),
     1AMIX(16),DL,TTMAX,SRISE,SRMIN,DELH,TDIL,NMIX
      COMMON /GEAR5/ IW1(81,9)/GEAR7/IW2(1500)
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART
      COMMON /MEXP/EXPMAX
      INTEGER SPECIS,HCSPEC,ALDSPC,PLSP,PSPEC,PLACE
C
C     SUN DATA
C
      DIMENSION X1(47),X2(47),X3(47),X4(47),X5(47),X6(47),
     &X7(47),X8(47),X9(47),X10(47),P1(31),P2(31),P3(31),P4(31)
     &,P5(31),P6(31),P7(31),P3(31),P9(31),P10(31),
     &S1(31),S2(31),S3(31),S4(31),S5(31),S6(31),S7(31),S8(31)
     &,S9(31),S10(31)
      EQUIVALENCE (XJ(1,1),X1(1)),(XJ(1,2),X2(1)),(XJ(1,3),X3(1)),
     &            (XJ(1,4),X4(1)),(XJ(1,5),X5(1)),(XJ(1,6),X6(1)),
     &            (XJ(1,7),X7(1)),(XJ(1,8),X8(1)),(XJ(1,9),X9(1)),
     &            (XJ(1,10),X10(1))
      EQUIVALENCE (SIGMO(1,1),S1(1)),(SIGMO(1,2),S2(1)),
     &            (SIGMO(1,3),S3(1)),(SIGMO(1,4),S4(1)),
     &            (SIGMO(1,5),S5(1)),(SIGMO(1,6),S6(1)),
     &            (SIGMO(1,7),S7(1)),(SIGMO(1,8),S8(1)),
     &            (SIGMO(1,9),S9(1)),(SIGMO(1,10),S10(1))
      EQUIVALENCE (PHI(1,1),P1(1)),(PHI(1,2),P2(1)),(PHI(1,3),P3(1)),
     &            (PHI(1,4),P4(1)),(PHI(1,5),P5(1)),(PHI(1,6),P6(1)),
     &            (PHI(1,7),P7(1)),(PHI(1,8),P8(1)),(PHI(1,9),P9(1)),
     &            (PHI(1,10),P10(1))
      DIMENSION KR1(200),KR2(200),KR3(200),KR4(200),KR5(200),
     *KR6(200),KR7(200)
      EQUIVALENCE (KR(1,1),KR1),(KR(1,2),KR2),(KR(1,3),KR3),
     &            (KR(1,4),KR4),(KR(1,5),KR5),(KR(1,6),KR6),
     &            (KR(1,7),KR7)
      DIMENSION IX1(200), IX2(200), IX3(200), IX4(60)
      EQUIVALENCE (IW2,IX1), (IW2(201),IX2), (IW2(401),IX3),
     &            (IW2(601),IX4)
      DIMENSION IW11(33),IW12(33),IW13(33),IW14(33),IW15(33),
     &          IW16(33),IW17(33),IW19(33)
      EQUIVALENCE (IW1(1,1),IW11),(IW1(1,2),IW12),(IW1(1,3),IW13),
     &            (IW1(1,4),IW14),(IW1(1,5),IW15),(IW1(1,6),IW16),
     &            (IW1(1,7),IW17),(IW1(1,9),IW19)
C
C   SUN DATA
C
```

```
                              BLOCK DATA
      DATA IPH/1,12,19,18,50,49,17,53,0/
      DATA KPH/9*0/
      DATA MAXL,MAXZ,MAXJ,LAM1,INC/09,10,47,2900,100/
      DATA Z/0.,10.,20.,30.,40.,50.,60.,70.,78.,86./
      DATA X1/
     & .0001500, .0398350, .4394000, .9551000,1.6132000,1.7134000,
     &1.8924000,1.9508000,2.3974000,2.3177000,2.3415000,3.1737000,
     &3.9935000,4.1186000,4.2224500,4.6172000,5.2089000,5.6146000,
     &5.7505000,5.7988000,5.7835500,5.8866000,5.9349500,5.9353000,
     &5.9797000,5.9271500,5.9095500,5.9687500,6.0576000,6.1739000,
     &6.2265000,6.2692500,6.3120000,6.3210000,6.3300000,6.4215000,
     &6.5130000,6.5937500,6.6745000,6.6590000,6.6435000,6.4600000,
     &6.4000000,6.3400000,6.2700000,6.2100000,6.1400000/
      DATA X2/
     & .0001500, .0380150, .4313000, .9438000,1.5944000,1.6964000,
     &1.8748000,1.9335000,2.3782000,2.3008000,2.3254000,3.1530000,
     &3.9685000,4.0949000,4.1180000,4.5120000,5.1817000,5.5851500,
     &5.7211000,5.7708000,5.7564500,5.8571500,5.9050500,5.9032000,
     &5.9503500,5.8983000,5.8814500,5.9396500,6.0280000,6.1445000,
     &6.1975000,6.2397500,6.2820000,6.2917500,6.3015000,6.3922500,
     &6.4830000,6.5630000,6.6430000,6.6265000,6.6100000,6.4500000,
     &6.3800000,6.3200000,6.2500000,6.1900000,6.1200000/
      DATA X3/
     & .0000000, .0325460, .4012000, .9006000,1.5384000,1.6450000,
     &1.8237000,1.8849000,2.3233000,2.2508000,2.2789000,3.0929000,
     &3.8957000,4.0250000,4.0509500,4.4421000,5.1007500,5.4983500,
     &5.6363000,5.6876500,5.6759000,5.7735000,5.8182500,5.8178500,
     &5.8656000,5.8161500,5.7972500,5.8528500,5.9412000,6.0576000,
     &6.1110000,6.1517500,6.1925000,6.2047500,6.2170000,6.3060000,
     &6.3950000,6.4720000,6.5490000,6.5367500,6.5245000,6.3500000,
     &6.2900000,6.2200000,6.1600000,6.1000000,6.0300000/
      DATA X4/
     & .0000000, .0246470, .3505500, .8261000,1.4402000,1.5547000,
     &1.7327000,1.7982000,2.2238000,2.1609000,2.1947000,2.9841000,
     &3.7652000,3.8985000,3.9301500,4.3168499,4.9576500,5.3444500,
     &5.4851000,5.5407500,5.5333000,5.6254000,5.6660000,5.6686000,
     &5.7171000,5.6701500,5.6504500,5.7025500,5.7869500,5.9047000,
     &5.9585000,5.9972500,6.0360000,5.9370000,5.8380000,6.0392500,
     &6.2405000,6.3142500,6.3880000,6.3787500,6.3695000,6.2000000,
     &6.1400000,6.0800000,6.0200000,5.9600000,5.9000000/
      DATA X5/
     & .0000000, .0155188, .2814000, .7174000,1.2922000,1.4160000,
     &1.5915000,1.6621000,2.0668000,2.0189000,2.0594000,2.8100000,
     &3.5559000,3.6956000,3.7348000,4.1135000,4.7279500,5.0991000,
     &5.2420000,5.3036000,5.3046500,5.3897000,5.4247000,5.4327000,
     &5.4816500,5.4392500,5.4197000,5.4671000,5.5507000,5.6665000,
     &5.7225000,5.7577500,5.7930000,5.6377500,5.4825000,5.7432500,
     &6.0040000,6.0740000,6.1440000,6.1392500,6.1345000,5.9800000,
     &5.9100000,5.8700000,5.8000000,5.7500000,5.6800000/
      DATA X6/
     & .0000000, .0074586, .1978000, .5706000,1.0832000,1.2153000,
     &1.3834000,1.4590000,1.8310000,1.8026000,1.8520000,2.5412000,
     &3.2319000,3.3780000,3.4279500,3.7932000,4.3661000,4.7150000,
     &4.8484500,4.9180000,4.9435500,5.0215500,5.0527000,5.0667000,
     &5.1156000,5.0801500,5.0612000,5.1035000,5.1827500,5.2964000,
     &5.3540000,5.3375000,5.4210000,5.4517500,5.4825000,5.5620000,
     &5.6415000,5.7032500,5.7750000,5.7772500,5.7795000,5.7100000,
     &5.6500000,5.6000000,5.5500000,5.4900000,5.4300000/
      DATA X7/
     & .0000000, .0022850, .1104300, .3890000, .8031000, .9357000,
     &1.2429000,1.1638000,1.4799000,1.4751000,1.5336000,2.1246000,
     &2.7246000,2.8754000,2.9379000,3.2742000,3.7832500,4.0991000,
     &4.2483000,4.3271000,4.3521500,4.4222500,4.4501500,4.4724000,
     &4.5209500,4.4947500,4.4787000,4.5142000,4.5850500,4.7142000,
     &4.7538500,4.7846750,4.8155000,4.8578000,4.9001000,4.9790500,
     &5.0580000,5.1225000,5.1870000,5.1992500,5.2115000,5.1500000,
     &5.1100000,5.0500000,5.0200000,4.9700000,4.9200000/
      DATA X8/
     & .0000000, .0003046, .0392490, .1937200, .4628000, .5726000,
     & .6841000, .7493000, .9722000, .9879000,1.0468000,1.4744000,
&1.9188000,2.0589000,2.1285500,2.4022500,2.7996500,3.0552500,
&3.1934500,3.2775000,3.3168000,3.3773000,3.4050000,3.4337500,
&3.4756000,3.4615500,3.4521000,3.4785500,3.5335500,3.6287000,
&3.6857000,3.7140000,3.7423000,3.7983500,3.8544000,3.9345500,
&4.0147000,4.0785750,4.1424500,4.1676250,4.1923000,4.0900000,
&4.0700000,4.0500000,4.0400000,4.0200000,4.0000000/
 DATA X9/
& .0000000, .0000000, .0092690, .0637200, .2029100, .2689000,
& .3276000, .3626000, .4767000, .4913000, .5291000, .7580000,
&1.0035000,1.0973000,1.1513500,1.3207000,1.5589500,1.7205500,
&1.8205500,1.8874500,1.9265000,1.9704500,1.9941500,2.0198000,
&2.0455000,2.0399500,2.0371500,2.0515500,2.0813000,2.1482000,
&2.1941000,2.2183000,2.2425000,2.3026500,2.3628000,2.4376250,
&2.5124500,2.5737000,2.6349500,2.6706250,2.7063000,2.7400000,
&2.7500000,2.7600000,2.7700000,2.7800000,2.7900000/
 DATA X10/
& .0000000, .0000000, .0009416, .0088930, .0389400, .0614900,
& .0765300, .0834100, .1065300, .1065000, .1113600, .1555700,
& .2017300, .2153800, .2226250, .2506650, .2921350, .3188350,
& .3330000, .3398000, .3416000, .3420500, .3394000, .3376000,
& .3312500, .3217000, .3147000, .3088500, .3034500, .3108000,
& .3201000, .3236750, .3272500, .3494500, .3716500, .4003750,
& .4291000, .4548250, .4805500, .4994500, .5184000, .5300000,
& .5400000, .5600000, .5600000, .5800000, .5900000/
 DATA S1/
& .852E-19, .128E-18, .183E-18, .247E-18, .310E-18, .374E-18,
& .449E-18, .501E-18, .541E-18, .570E-18, .582E-18, .595E-18,
& .580E-18, .545E-18, .515E-18, .485E-18, .455E-18,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    /
 DATA S2/
& .790E-20, .790E-20, .114E-19, .175E-19, .286E-19, .423E-19,
& .529E-19, .393E-19, .608E-19, .333E-19, .178E-19,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    /
 DATA S3/
& .162E-17, .444E-18, .119E-18, .336E-19, .879E-20, .194E-20,
& .386E-21,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    /
 DATA S4/
& .162E-17, .444E-18, .119E-18, .336E-19, .879E-20, .194E-20,
& .386E-21,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    /
 DATA S5/
& .318E-19, .325E-19, .315E-19, .234E-19, .237E-19, .198E-19,
& .837E-20, .176E-20,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    /
 DATA S6/
& .318E-19, .325E-19, .315E-19, .234E-19, .237E-19, .198E-19,
& .837E-20, .176E-20,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
&  .00    /
 DATA S7/
& .149E-19, .994E-20, .688E-20, .497E-20, .382E-20, .301E-20,
& .191E-20, .115E-20, .760E-21,  .00    ,  .00    ,  .00    ,
&  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,  .00    ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   /
 DATA S8/
& .466E-19, .409E-19, .296E-19, .169E-19, .692E-20, .134E-20,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   /
 DATA S9/
& .199E-21, .360E-21, .538E-21, .748E-21, .958E-21, .131E-20,
& .174E-20, .220E-20, .276E-20, .331E-20, .378E-20, .454E-20,
& .509E-20, .493E-20, .515E-20, .552E-20, .498E-20, .417E-20,
& .361E-20, .318E-20, .269E-20, .217E-20, .179E-20, .152E-20,
& .126E-20, .977E-21, .806E-21, .676E-21, .556E-21, .484E-21,
& .407E-21/
 DATA S10/
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   , .00   , .00   , .00   , .00   , .00   ,
& .00   /
 DATA P1/
& .988, .980, .972, .964, .956, .948,
& .940, .932, .924, .916, .908, .699,
& .175, .025, .006, .001, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000/
 DATA P2/
& .000,1.000,1.000,1.000,1.000,1.000,
&1.000,1.000,1.000,1.000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000/
 DATA P3/
& .000, .000,1.000,1.000,1.000,1.000,
&1.000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000/
 DATA P4/
&1.000,1.000,1.000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000/
 DATA P5/
& .810, .660, .520, .400, .290, .180,
& .090, .010, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000/
 DATA P6/
& .190, .340, .480, .600, .710, .820,
& .910, .990, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
& .000/
 DATA P7/
&1.000,1.000,1.000,1.000,1.000,1.000,
&1.000,1.000,1.000, .000, .000, .000,
& .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000/
      DATA P8/
     & .987, .722, .663, .474, .300, .123,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000/
      DATA P9/
     &1.000,1.000,1.000,1.000,1.000,1.000,
     &1.000,1.000,1.000,1.000,1.000,1.000,
     &1.000,1.000,1.000,1.000,1.000,1.000,
     &1.000,1.000,1.000,1.000,1.000,1.000,
     &1.000,1.000,1.000,1.000,1.000,1.000,
     &1.000/
      DATA P10/
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000, .000, .000, .000, .000, .000,
     & .000/
      DATA PSPEC/4HNO2 ,4HHONO,4HO3  ,4HO3  ,4HHCHO,4HHCHO,4HH2O2,4HALD2
     1,4HO3CH,4H    ,4H    /
      DATA MNLM/8*2900,4500,0,0/
      DATA MXLM/4500,3900,3500,3100,3600,3600,3700,3400,7500,0,0/
C
C    MECH DATA
C
      DATA NR/76/
      DATA KR1            /1,3,4,1,1,5,1,6,6,2,7,7,8,8,9,9,10,4,4,11,1
     11,8,4,12,13,13,13,13,13,14,12,12,24,24,2,2,2,2,2,27,28,20,18,27,28
     2,20,18,16,21,21,21,22,22,22,30,30,30,29,29,29,13,13,32,31,23,32,31
     3,23,26,19,25,17,15,32,31,23,124*0/
      DATA KR2            /0,0,2,4,3,2,5,0,0,1,7,0,1,2,2,9,0,0,0,0,0,4
     1,9,8,2,13,15,17,19,0,4,4,8,8,26,25,19,17,15,0,0,0,0,0,0,0,0,0,0,
     28,0,0,8,0,0,8,0,0,8,26,25,2,2,2,1,1,1,9,9,9,9,9,9,9,9,124*0/
      DATA KR3            /200*0/
      DATA KR4            /2,4,1,5,2,1,6,1,0,7,2,8,0,7,1,10,8,11,3,3,8
     1,9,8,13,14,14,14,14,14,21,8,8,25,26,1,1,1,1,1,21,22,21,21,29,9,30,
     222,21,0,9,9,0,15,23,0,17,31,0,19,32,14,14,19,17,15,135*0/
      DATA KR5            /3,4*0,1,0,5,0,7,1,2,0,0,8,0,8,0,0,0,8,0,0,0
     1,1,14,16,18,20,9,9,23,0,0,27,28,20,18,16,19,17,17,15,9,0,9,9,9,0,9
     2,0,0,9,0,0,9,0,0,9,0,27,28,1,1,1,135*0/
      DATA KR6            /29*0,22,22,21,168*0/
      DATA KR7            /200*0/
      DATA A/.35,4.4E+6,25.,.045,1.3E+4,1.3E+4,5600.,22.,.05,2.E-5,.001,
     1.018,8000.,3000.,1200.,8400.,8.4E-4,9.5E-4,.019,8.7E+10,1.E+10,84.
     2,2.4,2.5E+4,1000.,1.2E+4,1000.,1000.,1000.,1.E+5,.008,.008,1800.,1
     3800.,1800.,1200.,1800.,1800.,1200.,7.5E+4,1.E+5,8000.,4000.,1.5E+5
     4,3.E+5,1.E+5,8.E+4,8.E+4,.003,.001,1.5E+4,4.2E-6,9.8E-4,1.5E+4,6.E
     5-5,.0025,4.5E+4,6.E-5,.0019,4.5E+4,1000.,1000.,800.,800.,800.,100.
     6,100.,100.,8*4000.,124*0.0/
      DATA S/200*0./
      DATA ITYPE/1,1,2,2,2,2,2,1,1,2,2,1,2,2,2,2,1,1,1,1,1,2,2,2,2,2,2,2
     1,2,1,2,2,2,2,2,2,2,2,1,1,1,1,1,1,1,1,1,1,2,1,1,2,1,1,2,1,1,2,2
     2,15*2,124*0/
      DATA IA/1,12,34,38,50,54,57,61,79,93,95,98,106,120,124,131,134,141
     1,146,153,158,161,166,171,175,182,189,194,198,203,208,213,218,47*0/
      DATA JA/1,2,3,4,5,6,7,8,23,31,32,1,2,4,5,7,8,9,13,14,15,16,17,18,1
     19,20,23,25,26,27,28,31,32,1,2,3,4,1,2,3,4,5,8,9,11,12,21,22,23,1,2
     2,5,6,1,5,6,1,2,7,8,1,2,4,7,8,9,12,13,21,22,23,24,25,26,29,30,31,32
     3,1,2,4,8,9,10,15,17,19,23,25,26,31,32,8,10,3,8,11,4,8,9,12,13,21,2
     42,23,1,2,13,14,15,16,17,18,19,20,25,26,27,28,9,14,21,22,1,2,9,13,1
     54,15,16,9,16,21,1,2,9,13,14,17,18,9,15,18,21,22,1,2,9,13,14,19,20,
     69,17,20,21,30,8,9,21,8,9,15,22,23,1,2,9,15,23,8,24,25,26,1,2,9,13,
     714,25,28,1,2,9,13,14,26,27,9,19,21,27,29,9,17,22,28,8,9,19,29,32,8
     8,9,17,30,31,1,2,9,17,31,1,2,9,19,32,2283*0/
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      DATA SPECIS/4HNO2 ,4HNO  ,4HO   ,4HO3  ,4HNO3 ,4HN2O5,4HHONO,4HOH
     1 ,4HHO2 ,4HH2O2,4HO1D ,4HFROP,4HADD ,4HX   ,4HMEO2,4HMEO ,4HC2O2,4
     2HC2O ,4HC3O2,4HC3O ,4HHCHO,4HALD2,4HC2O3,4HBUT ,4HSCO2,4HC4O2,4HC4
     3O ,4HSCO ,4HALD4,4HALD3,4HC3O3,4HC4O3,4HM   ,48*4H    /
C
C   GEAR DATA
C
      DATA IW11             /6,10,5,7,11,24,3,16,29,30,28,31,32,18,12,19
     1,26,4,23,20,25,27,8,1,2,9,13,14,15,17,21,22,0/
      DATA IW12             /1,4,6,11,15,17,19,23,27,30,33,37,43,49,53,5
     16,63,69,76,84,88,94,98,112,130,147,170,179,187,194,202,211,218/
      DATA IW13             /1,3,4,6,9,11,14,17,19,23,27,30,34,38,42,49,
     155,61,69,73,79,86,94,103,111,118,124,129,133,136,138,139,139/
      DATA IW14             /1,3,4,6,9,11,14,17,19,23,27,30,34,38,42,49,
     155,61,69,73,79,86,94,95,96,97,98,99,100,101,102,102,0/
      DATA IW15             /1,3,4,7,10,11,12,14,17,19,21,24,29,34,37,39
     1,45,49,53,58,64,68,72,78,85,91,97,102,106,109,111,112,112/
      DATA IW16             /1,3,4,7,10,11,12,14,17,19,21,24,29,34,37,39
     1,45,49,53,58,64,68,72,78,85,91,97,102,106,109,111,111,0/
      DATA IW17             /3,4,6,9,11,14,17,19,23,27,29,34,38,41,48,55
     1,61,68,73,79,85,94,102,110,117,123,128,132,135,137,138,139,0/
      DATA IW19             /33,4*32,31,32,31,32,28,27,0,0,32,8*0,28,31,
     132,0,31,6*0/
      DATA IX1/1,3,24,2,26,1,3,18,24,25,4,23,24,25,5,18,6,23,5,7,18,24,8
     1,25,27,29,09,22,23,10,20,23,11,21,25,27,10,12,23,24,25,26,9,13,23,
     224,25,26,14,25,27,30,15,18,23,9,13,16,22,25,26,27,6,17,23,25,26,27
     3,7,15,18,23,24,25,26,15,18,19,23,24,25,26,32,16,20,25,27,6,21,23,2
     45,26,27,17,22,25,27,2,4,5,6,9,10,15,18,23,24,25,26,31,32,1,3,4,7,1
     52,13,16,17,18,19,21,23,24,25,26,27,29,30,3,4,7,12,13,16,17,18,19,2
     61,23,24,25,26,27,29,30,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,
     723,25,26,28,29,30,31,32,15,16,17,21,23,25,27,29,30,16,17,21,25,27,
     828,29,30,14,19,25,26,27,29,32,10,11,12,20,25,26,27/
      DATA IX2/30,8,14,15,18,20,22,23,28,31,11,14,15,18,23,28,32,3,24,23
     1,24,25,23,24,25,7,23,17,21,23,18,24,25,26,31,13,16,23,26,12,23,26,
     230,26,30,32,24,25,26,30,16,24,25,26,26,29,31,32,18,19,23,26,27,31,
     332,20,24,25,26,27,28,22,24,25,26,27,28,19,23,24,25,26,27,31,32,24,
     425,26,29,23,24,25,26,30,31,24,25,26,27,28,30,32,23,24,25,26,27,28,
     530,31,24,25,26,27,28,29,30,31,32,26,27,28,21,11,26,16,31,22,9,24,2
     65,18,4,23,26,15,27,31,32,19,6,21,17,9,10,12,13,24,25,7,18,3,1,4,23
     7,19,12,13,24,25,18,3,4,23,26,27,28,29,8,30,14,16,20,19,21,17,22,11
     8,12,13,24,25,18,23,26,2,29,30,16,19,21,17,12,13,24,25,27,28,29,8/
      DATA IX3/30,14,16,20,21,17,22,11,26,28,31,32,24,25,26,27,28,29,8,2
     14,25,26,27,28,30,14,23,26,31,23,26,29,32,19,231,210,109,225,3,24,2
     26,18,24,25,23,24,25,18,23,18,24,25,27,29,22,23,20,23,21,25,27,20,2
     33,24,25,26,22,23,24,25,26,25,27,30,18,23,22,23,24,25,26,27,23,25,2
     46,27,23,24,25,26,23,24,25,26,32,22,23,24,25,26,27,23,25,26,27,23,2
     55,26,27,24,25,26,27,31,32,25,26,27,29,30,31,32,26,27,29,30,31,32,2
     67,28,29,30,31,32,28,29,30,31,32,29,30,31,32,30,31,32,31,32,32,267,
     7188,205,228,255,102,73,256,189,254,223,232,230,76,172,237,191,276,
     8236,194,287,243,173,178,242,251,264,124,250,126,118,208,211,227,25
     93,229,190,259,129,260,258,82,280,294,195,286,265,84,186,104,197/
      DATA IX4/272,165,200,215,238,275,78,48,290,239,278,87,285,201,266,
     1284,77,135,72,288,300,291,95,137,92,246,158,249,292,159,162,161,30
     24,305,26*0/
C
C  SET DEFAULTS
C
      DATA HC/2.0/,XN/0.28/,NL/11/,MR/5/
      DATA ITTL/4HSTAN,4HDARD,4H OZO,4HNE I,4HSOPL,4HETH ,4HCOND,4HITIO,
     14HNS  ,9*4H    /
      DATA IOUT/6/,INFO/0/,NPTO/0/,NGO/1/
      DATA OZP/.08,.12,.16,.20,.24,.28,.30,.32,.34,.36,.40,9*0./
      DATA TSRT/0.0/,DTIM/420./,Z1/510./,Z2/630./,DCON/0.0/
      DATA SIG/1./,SIGMA/1./,RCTY/.25,.75,8*0./,FINHC/.1,.9,8*0./,XNF/.2
     15,.75/,ALDX/.02,.03,2*0./,ALDCRB/1.,2.,2*
     20./,FENX/.1,.9/,NI/0/,CARB/3.,4.,8*0./,FALHC/.10000000,.900,8*0./
      DATA NEM/0/,BMIX(1)/-3./,MMIX/0/,EMHC(1)/-3./,EMNOX(1)/-3./
      DATA DSTRT/800./,DEND/1800./,PLTGRD/0./,OHC/0./,FCTR/0.6/
      DATA TICZ/0.07/,DIGZ/0.10/,CHRZ/0.10/,HC1/8.5/,XN1/5.95/
      DATA CHRSIZ/0.07/
```

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                        BLOCK DATA
DATA FD/0.,.07,.14,.33,.50,.70/                                     AV 421
DATA AMC/32.7892,10.9811,-26.3876,7.4405,3.4242/                    AV 422
DATA BMC/0.0,6.8857,9.1918,-5.8492,-2.0545/                         AV 423
DATA CMC/.1251,.6071,1.7325,2.3676,1.0239/                          AV 424
DATA FG/0.,.02,.10,.58,.85,1.0/                                     AV 425
DATA IP/8/,RFCT/9*1./,NS/33/,KOZ/4/,PLSP/4HO3  /                    AV 426
DATA KFACT/0/                                                       AV 427
DATA HCSPEC/4HPROP,4HBUT ,8*4H    /,ALDSPC/4HHCHO,4HALD2,2*4H    / AV 428
DATA IH/12,24,8*0/,IALD/21,22,2*0/,INOX/1,2/,NHC/2/,NALD/2/         AV 429
DATA OZIN/0./,OZAL/0./,HCIN/0./,HCAL/0./,XNIN/0./,XNAL/0./          AV 430
DATA ERR/0.01/,TEMP/303.0/                                          AV 431
DATA ESTOP/0.0/,STOPP/600./,TPRNT/60./,TSTEP/60./                   AV 432
DATA PLACE/4H LOS,4H ANG,4HELES,4H, CA,4HLIF.,4H    /               AV 433
DATA SLA/34.058/,SLO/118.250/,TZ/8.0/,IY/1975/,IM/6/,ID/21/         AV 434
DATA IN/5/                                                          AV 435
DATA JSTRT/0800/,JSTOP/1900/,IINC/60/,TSTART/480./                  AV 436
DATA UROUND/7.5E-9/                                                 AV 437
DATA EXPMAX/87.4/                                                   AV 438
DATA NSPARS/1/                                                      AV 439
END                                                                 AV 440-
```